Dieter A. Wolf-Gladrow

Lattice-Gas Cellular Automata and Lattice Boltzmann Models

An Introduction

Springer

Table of Contents

1. Introduction	1
1.1 Preface	2
1.2 Overview	4
1.3 The basic idea of lattice-gas cellular automata and lattice Boltzmann models	7
1.3.1 The Navier-Stokes equation	7
1.3.2 The basic idea	9
1.3.3 Top-down versus bottom-up	11
1.3.4 LGCA versus molecular dynamics	11
2. Cellular Automata	15
2.1 What are cellular automata?	15
2.2 A short history of cellular automata	16
2.3 One-dimensional cellular automata	17
2.3.1 Qualitative characterization of one-dimensional cellular automata	23
2.4 Two-dimensional cellular automata	29
2.4.1 Neighborhoods in 2D	29
2.4.2 Fredkin's game	30
2.4.3 'Life'	31
2.4.4 CA: what else? Further reading	35
2.4.5 From CA to LGCA	36

3. Lattice-gas cellular automata	39
3.1 The HPP lattice-gas cellular automata	39
3.1.1 Model description	39
3.1.2 Implementation of the HPP model: How to code lattice-gas cellular automata?	44
3.1.3 Initialization	48
3.1.4 Coarse graining	50
3.2 The FHP lattice-gas cellular automata	53
3.2.1 The lattice and the collision rules	53
3.2.2 Microdynamics of the FHP model	59
3.2.3 The Liouville equation	64
3.2.4 Mass and momentum density	65
3.2.5 Equilibrium mean occupation numbers	66
3.2.6 Derivation of the macroscopic equations: multi-scale analysis	69
3.2.7 Boundary conditions	79
3.2.8 Inclusion of body forces	80
3.2.9 Numerical experiments with FHP	83
3.2.10 The 8-bit FHP model	87
3.3 Lattice tensors and isotropy in the macroscopic limit	90
3.3.1 Isotropic tensors	90
3.3.2 Lattice tensors: single-speed models	91
3.3.3 Generalized lattice tensors for multi-speed models	95
3.3.4 Thermal LBMs: D2Q13-FHP (multi-speed FHP model)	101
3.3.5 Exercises	104
3.4 Desperately seeking a lattice for simulations in three dimen- sions	105
3.4.1 Three dimensions	105
3.4.2 Five and higher dimensions	108
3.4.3 Four dimensions	109
3.5 FCHC	113
3.5.1 Isometric collision rules for FCHC by Hénon	113
3.5.2 FCHC, computers and modified collision rules	114
3.5.3 Isometric rules for HPP and FHP	115

3.5.4	What else?	116
3.6	The pair interaction (PI) lattice-gas cellular automata	118
3.6.1	Lattice, cells, and interaction in 2D	118
3.6.2	Macroscopic equations	121
3.6.3	Comparison of PI with FHP and FCHC	124
3.6.4	The collision operator and propagation in C and FOR-TRAN	124
3.7	Multi-speed and thermal lattice-gas cellular automata	128
3.7.1	The D3Q19 model	128
3.7.2	The D2Q9 model	131
3.7.3	The D2Q21 model	134
3.7.4	Transsonic and supersonic flows: D2Q25, D2Q57, D2Q129	134
3.8	Zanetti ('staggered') invariants	135
3.8.1	FHP	135
3.8.2	Significance of the Zanetti invariants	135
3.9	Lattice-gas cellular automata: What else?	137
4.	Some statistical mechanics	139
4.1	The Boltzmann equation	139
4.1.1	Five collision invariants and Maxwell's distribution ...	140
4.1.2	Boltzmann's H-theorem	141
4.1.3	The BGK approximation	143
4.2	Chapman-Enskog: From Boltzmann to Navier-Stokes	145
4.2.1	The conservation laws	146
4.2.2	The Euler equation	147
4.2.3	Chapman-Enskog expansion	147
4.3	The maximum entropy principle	153
5.	Lattice Boltzmann Models	159
5.1	From lattice-gas cellular automata to lattice Boltzmann models	159
5.1.1	Lattice Boltzmann equation and Boltzmann equation .	160
5.1.2	Lattice Boltzmann models of the first generation	163
5.2	BGK lattice Boltzmann model in 2D	165

Table of Contents

5.2.1	Derivation of the W_i	170
5.2.2	Entropy and equilibrium distributions	171
5.2.3	Derivation of the Navier-Stokes equations by multi-scale analysis	174
5.2.4	Storage demand	182
5.2.5	Simulation of two-dimensional decaying turbulence ...	183
5.2.6	Boundary conditions for LBM	189
5.3	Hydrodynamic lattice Boltzmann models in 3D	195
5.3.1	3D-LBM with 19 velocities	195
5.3.2	3D-LBM with 15 velocities and Koelman distribution .	196
5.3.3	3D-LBM with 15 velocities proposed by Chen et al. (D3Q15)	197
5.4	Equilibrium distributions: the ansatz method	198
5.4.1	Multi-scale analysis	199
5.4.2	Negative distribution functions at high speed of sound	203
5.5	Hydrodynamic LBM with energy equation	205
5.6	Stability of lattice Boltzmann models	208
5.6.1	Nonlinear stability analysis of uniform flows	208
5.6.2	The method of linear stability analysis (von Neumann)	210
5.6.3	Linear stability analysis of BGK lattice Boltzmann models	212
5.6.4	Summary	215
5.7	Simulating ocean circulation with LBM	219
5.7.1	Introduction	219
5.7.2	The model of Munk (1950)	219
5.7.3	The lattice Boltzmann model	222
5.8	A lattice Boltzmann equation for diffusion	232
5.8.1	Finite differences approximation	232
5.8.2	The lattice Boltzmann model for diffusion	233
5.8.3	Multi-scale expansion	234
5.8.4	The special case $\omega = 1$	236
5.8.5	The general case	236
5.8.6	Numerical experiments	236
5.8.7	Summary and conclusion	237

5.8.8	Diffusion equation with a diffusion coefficient depending on concentration	240
5.8.9	Further reading	242
5.9	Lattice Boltzmann model: What else?	243
5.10	Summary and outlook	245
6.	Appendix	247
6.1	Boolean algebra	248
6.2	FHP: After some algebra one finds	250
6.3	Coding of the collision operator of FHP-II and FHP-III in C ..	254
6.4	Thermal LBM: derivation of the coefficients	258
6.5	Schläfli symbols	264
6.6	Notation, symbols and abbreviations	266