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 dimensions 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 FORTRAN ... 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

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