Contents

1 Introduction 1
1.1 Ideas and References 1
1.2 Content and Reading Approaches 11

2 The Source of Examples 21
2.1 The Boltzmann Equation 21
2.1.1 The Equation 21
2.1.2 The Basic Properties of the Boltzmann Equation 23
2.1.3 Linearized Collision Integral 25
2.2 Phenomenology and Quasi-Chemical Representation of the Boltzmann Equation 26
2.3 Kinetic Models 27
2.4 Methods of Reduced Description 28
2.4.1 The Hilbert Method 29
2.4.2 The Chapman–Enskog Method 30
2.4.3 The Grad Moment Method 32
2.4.4 Special Approximations 33
2.4.5 The Method of Invariant Manifold 33
2.4.6 Quasiequilibrium Approximations 35
2.5 Discrete Velocity Models 36
2.6 Direct Simulation 36
2.7 Lattice Gas and Lattice Boltzmann Models 37
2.7.1 Discrete Velocity Models for Hydrodynamics 37
2.7.2 Entropic Lattice Boltzmann Method 42
2.7.3 Entropic Lattice BGK Method (ELBGK) 42
2.7.4 Boundary Conditions 46
2.7.5 Numerical Illustrations of the ELBGK 46
2.8 Other Kinetic Equations 46
2.8.1 The Enskog Equation for Hard Spheres 46
2.8.2 The Vlasov Equation 48
2.8.3 The Fokker–Planck Equation 49
2.9 Equations of Chemical Kinetics and Their Reduction 50
2.9.1 Dissipative Reaction Kinetics 50

2.9.2 The Problem of Reduced Description in Chemical Kinetics . . . 55
2.9.3 Partial Equilibrium Approximations . . . 55
2.9.4 Model Equations . . . 57
2.9.5 Quasi-Steady State Approximation . . . 59
2.9.6 Thermodynamic Criteria for the Selection of Important Reactions . . . 61
2.9.7 Opening . . . 62

3 Invariance Equation in Differential Form . . . 65

4 Film Extension of the Dynamics: Slowness as Stability . . . 69
4.1 Equation for the Film Motion . . . 69
4.2 Stability of Analytical Solutions . . . 71

5 Entropy, Quasiequilibrium, and Projectors Field . . . 79
5.1 Moment Parameterization . . . 79
5.2 Entropy and Quasiequilibrium . . . 80
5.3 Thermodynamic Projector without a Priori Parameterization . . . 85
5.4 Uniqueness of Thermodynamic Projector . . . 87
5.4.1 Projection of Linear Vector Field . . . 87
5.4.2 The Uniqueness Theorem . . . 88
5.4.3 Orthogonality of the Thermodynamic Projector and Entropic Gradient Models . . . 90
5.4.4 Violation of the Transversality Condition, Singularity of Thermodynamic Projection, and Steps of Relaxation . . . 92
5.4.5 Thermodynamic Projector, Quasiequilibrium, and Entropy Maximum . . . 93
5.5 Example: Quasiequilibrium Projector and Defect of Invariance for the Local Maxwellians Manifold of the Boltzmann Equation . . . 97
5.5.1 Difficulties of Classical Methods of the Boltzmann Equation Theory . . . 98
5.5.2 Boltzmann Equation . . . 99
5.5.3 Local Manifolds . . . 100
5.5.4 Thermodynamic Quasiequilibrium Projector . . . 101
5.5.5 Defect of Invariance for the LM Manifold . . . 102
5.6 Example: Quasiequilibrium Closure Hierarchies for the Boltzmann Equation . . . 103
5.6.1 Triangle Entropy Method . . . 103
5.6.2 Linear Macroscopic Variables . . . 106

5.6.3 Transport Equations for Scattering Rates in the Neighbourhood of Local Equilibrium. Second and Mixed Hydrodynamic Chains 113
5.6.4 Distribution Functions of the Second Quasiequilibrium Approximation for Scattering Rates 116
5.6.5 Closure of the Second and Mixed Hydrodynamic Chains 123
5.6.6 Appendix: Formulas of the Second Quasiequilibrium Approximation of the Second and Mixed Hydrodynamic Chains for Maxwell Molecules and Hard Spheres 126
5.7 Example: Alternative Grad Equations and a "New Determination of Molecular Dimensions" (Revisited) 131
5.7.1 Nonlinear Functionals Instead of Moments in the Closure Problem 132
5.7.2 Linearization 133
5.7.3 Truncating the Chain 134
5.7.4 Entropy Maximization 134
5.7.5 A New Determination of Molecular Dimensions (Revisited) 136

6 Newton Method with Incomplete Linearization 139
6.1 The Method 139
6.2 Example: Two-Step Catalytic Reaction 141
6.3 Example: Non-Perturbative Correction of Local Maxvellian Manifold and Derivation of Nonlinear Hydrodynamics from Boltzmann Equation (1D) 144
6.3.1 Positivity and Normalization 144
6.3.2 Galilean Invariance of Invariance Equation 145
6.3.3 Equation of the First Iteration 146
6.3.4 Parametrix Expansion 149
6.3.5 Finite-Dimensional Approximations to Integral Equations 154
6.3.6 Hydrodynamic Equations 159
6.3.7 Nonlocality 160
6.3.8 Acoustic Spectra 160
6.3.9 Nonlinearity 161
6.4 Example: Non-Perturbative Derivation of Linear Hydrodynamics from the Boltzmann Equation (3D) 163

6.5 Example: Dynamic Correction to Moment Approximations 170
6.5.1 Dynamic Correction or Extension of the List of Variables? 170
6.5.2 Invariance Equation for Thirteen-Moment Parameterization 171
6.5.3 Solution of the Invariance Equation 174
6.5.4 Corrected Thirteen-Moment Equations 175
6.5.5 Discussion: Transport Coefficients, Destroying the Hyperbolicity, etc. 177

7 Quasi-Chemical Representation 179
7.1 Decomposition of Motions, Non-Uniqueness of Selection of Fast Motions, Self-Adjoint Linearization, Onsager Filter, and Quasi-Chemical Representation 179
7.2 Example: Quasi-Chemical Representation and Self-Adjoint Linearization of the Boltzmann Collision Operator 183

8 Hydrodynamics From Grad's Equations: What Can We Learn From Exact Solutions? 189
8.1 The "Ultra-Violet Catastrophe" of the Chapman-Enskog Expansion 189
8.2 The Chapman–Enskog Method for Linearized Grad's Equations 192
8.3 Exact Summation of the Chapman–Enskog Expansion 195
8.3.1 The $1D10M$ Grad Equations 195
8.3.2 The $3D10M$ Grad Equations 202
8.4 The Dynamic Invariance Principle 212
8.4.1 Partial Summation of the Chapman–Enskog Expansion 212
8.4.2 The Dynamic Invariance 215
8.4.3 The Newton Method 217
8.4.4 Invariance Equation for the $1D13M$ Grad System 223
8.4.5 Invariance Equation for the $3D13M$ Grad System 228
8.4.6 Gradient Expansions in Kinetic Theory of Phonons . . . 230
8.4.7 Nonlinear Grad Equations 239
8.5 The Main Lesson 246

9 Relaxation Methods 247
9.1 "Large Stepping" for the Equation of the Film Motion 247
9.2 Example: Relaxation Method for the Fokker-Planck Equation 248

9.2.1 Quasi-Equilibrium Approximations for the Fokker-Planck Equation . . . 248
9.2.2 The Invariance Equation for the Fokker-Planck Equation . . . 251
9.2.3 Diagonal Approximation . . . 252
9.3 Example: Relaxational Trajectories: Global Approximations . . . 254
9.3.1 Initial Layer and Large Stepping . . . 254
9.3.2 Extremal Properties of the Limiting State . . . 256
9.3.3 Approximate Trajectories . . . 259
9.3.4 Relaxation of the Boltzmann Gas . . . 262
9.3.5 Estimations . . . 268
9.3.6 Discussion . . . 276

10 Method of Invariant Grids . . . 279
10.1 Invariant Grids . . . 279
10.2 Grid Construction Strategy . . . 282
10.2.1 Growing Lump . . . 282
10.2.2 Invariant Flag . . . 282
10.2.3 Boundaries Check and the Entropy . . . 283
10.3 Instability of Fine Grids . . . 283
10.4 Which Space is Most Appropriate for the Grid Construction? . . . 284
10.5 Carleman's Formula in the Analytical Invariant Manifolds Approximations. First Benefit of Analyticity: Superresolution . . . 285
10.6 Example: Two-Step Catalytic Reaction . . . 287
10.7 Example: Model Hydrogen Burning Reaction . . . 291
10.8 Invariant Grid as a Tool for Data Visualization . . . 295

11 Method of Natural Projector . . . 299
11.1 Ehrenfests' Coarse-Graining Extended to a Formalism of Nonequilibrium Thermodynamics . . . 299
11.2 Example: From Reversible Dynamics to Navier–Stokes and Post-Navier–Stokes Hydrodynamics by Natural Projector . . . 301
11.2.1 General Construction . . . 303
11.2.2 Enhancement of Quasiequilibrium Approximations for Entropy-Conserving Dynamics . . . 304
11.2.3 Entropy Production . . . 307
11.2.4 Relation to the Work of Lewis . . . 308
11.2.5 Equations of Hydrodynamics . . . 310
11.2.6 Derivation of the Navier–Stokes Equations . . . 310
11.2.7 Post-Navier–Stokes Equations . . . 313

11.3 Example: Natural Projector
for the Mc Kean Model 316
11.3.1 General Scheme 316
11.3.2 Natural Projector for Linear Systems 318
11.3.3 Explicit Example of the Fluctuation–Dissipation
Formula 319
11.3.4 Comparison with the Chapman–Enskog Method
and Solution of the Invariance Equation 321

**12 Geometry of Irreversibility:
The Film of Nonequilibrium States** 325
12.1 The Thesis About Macroscopically Definable Ensembles
and the Hypothesis About
Primitive Macroscopically Definable Ensembles 325
12.2 The Problem of Irreversibility 328
12.2.1 The Phenomenon of the Macroscopic Irreversibility . . . 328
12.2.2 Phase Volume and Dynamics of Ensembles 329
12.2.3 Macroscopically Definable Ensembles
and Quasiequilibria 331
12.2.4 Irreversibility and Initial Conditions 334
12.2.5 Weak and Strong Tendency to Equilibrium,
Shaking and Short Memory 335
12.2.6 Subjective Time and Irreversibility 336
12.3 Geometrization of Irreversibility 336
12.3.1 Quasiequilibrium Manifold 336
12.3.2 Quasiequilibrium Approximation 339
12.4 Natural Projector
and Models of Nonequilibrium Dynamics 341
12.4.1 Natural Projector 341
12.4.2 One-Dimensional Model of Nonequilibrium States 343
12.4.3 Curvature and Entropy Production:
Entropic Circle and First Kinetic Equations 346
12.5 The Film of Non-Equilibrium States 348
12.5.1 Equations for the Film 348
12.5.2 Thermodynamic Projector on the Film 349
12.5.3 Fixed Points of the Film Equation 352
12.5.4 The Failure of the Simplest
Galerkin-Type Approximations
for Conservative Systems 353
12.5.5 Second Order Kepler Models of the Film 355
12.5.6 The Finite Models: Termination at the Horizon Points 356
12.5.7 The Transversal Restart Lemma 359
12.5.8 The Time Replacement, and the Invariance
of the Projector 360
12.5.9 Correction to the Infinite Models 360

12.5.10 The Film, and the Macroscopic Equations 361
12.5.11 New in the Separation of the Relaxation Times 363
12.6 The Main Results 364

13 Slow Invariant Manifolds for Open Systems 367
13.1 Slow Invariant Manifold for a Closed System Has Been Found. What Next? 367
13.2 Slow Dynamics in Open Systems. Zero-Order Approximation and the Thermodynamic Projector 368
13.3 Slow Dynamics in Open Systems. First-Order Approximation 371
13.4 Beyond the First-Order Approximation: Higher-Order Dynamic Corrections, Stability Loss and Invariant Manifold Explosion 373
13.5 Example: The Universal Limit in Dynamics of Dilute Polymeric Solutions 375
13.5.1 The Problem of Reduced Description in Polymer Dynamics 377
13.5.2 The Method of Invariant Manifold for Weakly Driven Systems 382
13.5.3 Linear Zero-Order Equations 387
13.5.4 Auxiliary Formulas. 1. Approximations to Eigenfunctions of the Fokker–Planck Operator . . . 388
13.5.5 Auxiliary Formulas. 2. Integral Relations 390
13.5.6 Microscopic Derivation of Constitutive Equations . . . 391
13.5.7 Tests on the FENE Dumbbell Model 397
13.5.8 The Main Results of this Example are as Follows: . . 401
13.6 Example: Explosion of Invariant Manifold, Limits of Macroscopic Description for Polymer Molecules, Molecular Individualism, and Multimodal Distributions 403
13.6.1 Dumbbell Models and the Problem of the Classical Gaussian Solution Stability 403
13.6.2 Dynamics of the Moments and Explosion of the Gaussian Manifold 405
13.6.3 Two-Peak Approximation for Polymer Stretching in Flow and Explosion of the Gaussian Manifold . . . 407
13.6.4 Polymodal Polyhedron and Molecular Individualism 411

14 Dimension of Attractors Estimation 419
14.1 Lyapunov Norms, Finite-Dimensional Asymptotics and Volume Contraction 419
14.2 Examples: Lyapunov Norms for Reaction Kinetics 423

14.3 Examples: Infinite-Dimensional Systems With Finite-Dimensional Attractors 426
14.4 Systems with Inheritance: Dynamics of Distributions with Conservation of Support, Natural Selection and Finite-Dimensional Asymptotics 432
14.4.1 Introduction: Unusual Conservation Law 432
14.4.2 Optimality Principle for Limit Diversity 436
14.4.3 How Many Points Does the Limit Distribution Support Hold? 438
14.4.4 Selection Efficiency 440
14.4.5 Gromov's Interpretation of Selection Theorems 444
14.4.6 Drift Equations 445
14.4.7 Three Main Types of Stability 449
14.4.8 Main Results About Systems with Inheritance 450
14.5 Example: Cell Division Self-Synchronization 451

15 Accuracy Estimation and Post-Processing in Invariant Manifolds Construction 457
15.1 Formulas for Dynamic and Static Post-Processing 457
15.2 Example: Defect of Invariance Estimation and Switching from the Microscopic Simulations to Macroscopic Equations 460
15.2.1 Invariance Principle and Micro-Macro Computations 460
15.2.2 Application to Dynamics of Dilute Polymer Solution 461

16 Conclusion 467

References 469

Mathematical Notation and Some Terminology 491

Index 493