

Contents

| | |
|---|-----------|
| Preface | 5 |
| 1 Getting started | 9 |
| 1.1 Introductory remarks | 9 |
| 1.2 Intermolecular potential models | 10 |
| 1.3 Mimicking an infinite system | 14 |
| 2 Basics of molecular dynamics | 17 |
| 2.1 General remarks | 17 |
| 2.2 Verlet method | 19 |
| 2.3 Predictor-corrector algorithms | 20 |
| 2.4 Few technical remarks | 21 |
| 3 Basics of Monte Carlo method | 23 |
| 3.1 Naive versus smart sampling | 23 |
| 3.2 Metropolis algorithm | 25 |
| 3.3 Acceptance ratio | 29 |
| 4 Measurements | 31 |
| 4.1 Thermodynamic properties | 32 |
| 4.1.1 Mechanical quantities | 32 |
| 4.1.2 Entropic quantities | 34 |
| 4.2 Structural properties | 37 |
| 4.3 Auxiliary quantities | 42 |
| 4.4 Estimation of errors | 43 |
| 5 Implementation of simulations | 45 |
| 5.1 MD versus MC method | 45 |

| | | |
|----------|--|-----------|
| 5.2 | Initial configuration | 46 |
| 5.3 | System size and cut-off potentials | 48 |
| 5.3.1 | Fast decaying potentials | 50 |
| 5.3.2 | Slowly decaying (long-range) potentials | 52 |
| 5.4 | Molecular systems | 53 |
| 5.4.1 | Rigid molecules | 54 |
| 5.4.2 | Flexible molecules | 55 |
| 5.4.3 | Orientalional order parameter | 59 |
| 6 | Simulations at various conditions | 61 |
| 6.1 | MC simulations at constant pressure | 61 |
| 6.2 | Grandcanonical ensemble | 64 |
| 6.3 | MD at constant temperature | 66 |
| 7 | Phases at equilibrium | 69 |
| 7.1 | Gibbs ensemble | 70 |
| 7.2 | Phase equilibria with explicit interface | 72 |
| 7.3 | Gibbs-Duhem integration | 73 |
| 8 | Appendix | 77 |
| 8.1 | Basic thermodynamic relations | 77 |
| 8.2 | Basic statistical-mechanical expressions | 78 |
| 8.3 | Additional readings | 81 |