

# Contents

|  |    |
|--|----|
| <i>Preface</i>   | v  |
| 1. Mathematical, Physical, and Computational Preliminaries | 1  |
| 1.1. The N-Body Problem . . . . .                          | 1  |
| 1.2. Classical Molecular Potentials . . . . .              | 1  |
| 1.3. Molecular Mechanics . . . . .                         | 4  |
| 1.4. The Leap Frog Formulas . . . . .                      | 4  |
| 1.5. Turbulence . . . . .                                  | 8  |
| 1.5.1. Engineering . . . . .                               | 9  |
| 1.5.2. Theoretical . . . . .                               | 9  |
| 1.5.3. Numerical . . . . .                                 | 10 |
| 1.6. Overview . . . . .                                    | 11 |
| 2. Molecular Cavity Flow of Argon Vapor in Two Dimensions  | 13 |
| 2.1. Introduction . . . . .                                | 13 |
| 2.2. Equations of Motion for Argon Vapor . . . . .         | 14 |
| 2.3. The Cavity Problem . . . . .                          | 15 |
| 2.4. Computational Considerations . . . . .                | 16 |
| 2.5. Examples of Primary Vortex Generation . . . . .       | 17 |
| 2.6. Example of Turbulent Flow . . . . .                   | 22 |
| 2.7. Remarks . . . . .                                     | 29 |
| 2.8. The Fortran Program ARGON.FOR . . . . .               | 29 |
| 2.9. The Fortran Program YOUWIN.FOR . . . . .              | 32 |

|       |  |     |
|-------|--|-----|
| 3.    | Molecular Cavity Flow of Air Vapor in Two Dimensions     | 37  |
| 3.1.  | Molecular Formulas . . . . .                             | 37  |
| 3.2.  | The Cavity Problem . . . . .                             | 38  |
| 3.3.  | Initial Data . . . . .                                   | 38  |
| 3.4.  | Examples of Primary Vortex Generation . . . . .          | 39  |
| 3.5.  | Turbulent Flow . . . . .                                 | 44  |
| 3.6.  | The Fortran Program AIR.FOR . . . . .                    | 51  |
| 4.    | Molecular Cavity Flow of Water Vapor in Two Dimensions   | 55  |
| 4.1.  | Introduction . . . . .                                   | 55  |
| 4.2.  | Equations of Motion for Water Vapor Molecules . . . . .  | 55  |
| 4.3.  | Examples of Primary Vortex Generation . . . . .          | 57  |
| 4.4.  | Example of Turbulent Flow . . . . .                      | 60  |
| 4.5.  | A Speculative Study of Liquid Water . . . . .            | 65  |
| 4.6.  | The Fortran Program CAV.FOR . . . . .                    | 70  |
| 5.    | Molecular Cavity Flow of Water Vapor in Three Dimensions | 75  |
| 5.1.  | Introduction . . . . .                                   | 75  |
| 5.2.  | Molecular Arrangement and the Cavity Problem . . . . .   | 76  |
| 5.3.  | Computational Considerations . . . . .                   | 78  |
| 5.4.  | Examples . . . . .                                       | 78  |
| 5.5.  | Turbulent Flow . . . . .                                 | 87  |
| 5.6.  | The Fortran program CAV3D.FOR. . . . .                   | 95  |
| 6.    | Particle Models of Flow in Two Dimensions                | 99  |
| 6.1.  | Introduction . . . . .                                   | 99  |
| 6.2.  | Particle Arrangement and Equations . . . . .             | 99  |
| 6.3.  | Particle Equilibrium . . . . .                           | 103 |
| 6.4.  | Examples . . . . .                                       | 103 |
| 6.5.  | Turbulence . . . . .                                     | 108 |
| 6.6.  | Heating Water Vapor in a Square Cavity . . . . .         | 112 |
| 6.7.  | A Speculative Study of Liquid Water . . . . .            | 114 |
| 6.8.  | Particle Equations of Motion . . . . .                   | 118 |
| 6.9.  | Particle Equilibrium . . . . .                           | 121 |
| 6.10. | Primary Vortex Generation . . . . .                      | 122 |
| 6.11. | Turbulence . . . . .                                     | 129 |
| 6.12. | The Fortran Program PARTICLE.FOR . . . . .               | 133 |

|      |  |     |
|------|--|-----|
| 7.   | The Flow of Water Vapor Around a Flat Plate            | 137 |
| 7.1. | Introduction . . . . .                                 | 137 |
| 7.2. | Mathematical and Physical Preliminaries . . . . .      | 137 |
| 7.3. | Approximate Equations . . . . .                        | 138 |
| 7.4. | Problem Formulation . . . . .                          | 139 |
| 7.5. | Examples . . . . .                                     | 141 |
| 7.6. | Remarks . . . . .                                      | 150 |
| 7.7. | The Fortran Program PLATE.FOR . . . . .                | 152 |
| 8.   | Extant Problems with Continuum Models                  | 155 |
| 8.1. | Introduction . . . . .                                 | 155 |
| 8.2. | Concepts of Infinity . . . . .                         | 155 |
| 8.3. | The Surface Area Paradox . . . . .                     | 157 |
| 8.4. | Paradoxes of Zeno . . . . .                            | 159 |
| 8.5. | A Nonsolvable Problem in Population Genetics . . . . . | 160 |
| 8.6. | Time as a Continuum in Fluid Dynamics . . . . .        | 161 |
| 8.7. | Remark . . . . .                                       | 161 |
|      | <i>References and Additional Sources</i>               | 163 |
|      | <i>Index</i>   | 167 |