CONTENTS

Foreword xv

Preface to the Paperback Edition xvii

Preface xix

Chapter 1 Computer Experiments Using Particle Models 1

1-1 Introduction 1
1-2 The Computer Experiment 2
1-2-1 The Role of the Computer Experiment 2
1-2-2 Setting Up Computer Experiments 4
1-3 Length and Time Scales 6
1-4 Physical Systems 9
1-4-1 Correlated Systems 10
1-4-2 Uncorrelated (Collisionless) Systems 13
1-4-3 Collisional Systems 14
1-4-4 Collision-Dominated Systems 15
1-5 Particle Models 18
1-5-1 The Particle-Particle Method 18
1-5-2 The Particle-Mesh Method 21
1-5-3 The Particle-Particle–Particle-Mesh Method 22

Chapter 2 A One-Dimensional Plasma Model 24

2-1 The Physical System 24

2-2 Discretization of the Mathematical Model 26
2-2-1 The Superparticle Equations 26
2-2-2 The Field Equations 28
2-2-3 Charge Assignment and Force Interpolation 30
2-2-4 The Discrete Model 31
2-3 Numerical Algorithms 32
2-3-1 Dimensionless Units 33
2-3-2 Charge Assignment 34
2-3-3 Poisson's Equation 35
2-4 Computer Experiments 38
2-4-1 The Two-Particle Test 38
2-4-2 Wave Dispersion 40
2-4-3 The Cold Plasma 42
2-4-4 Energy Conservation 42
2-4-5 The Two-Stream Instability 42

Chapter 3 The Simulation Program 44

3-1 Introduction 44
3-2 Program Requirements and Specification 45
3-2-1 User's Requirements 45
3-2-2 Program Specifications 47
3-3 The OLYMPUS Programming System 48
3-4 The Program ES1D1V 58
3-4-1 The Program Control Structure 60
3-4-2 The Master Index 62
3-4-3 Class 1: The Prologue Subprograms 90
3-4-4 Calculation and Output Subprograms 91
3-5 Final Remarks 92

Chapter 4 Time Integration Schemes 94

4-1 Introduction 94
4-2 Consistency 95
4-3 Accuracy 96
4-4 Stability 97
4-4-1 The Root Locus Method 100
4-4-2 The Amplification Matrix 104
4-5 Efficiency 106
4-6 The Leapfrog Harmonic Oscillator 107
4-7 Examples of Integration Schemes 111
4-7-1 Lorentz Force Integrators 111
4-7-2 Viscous Force Integrators 114
4-7-3 Low-Storage Runge–Kutta Schemes 117

Chapter 5 The Particle-Mesh Force Calculation 120

5-1 Introduction 120
5-2 Forces in One Dimension 121
5-2-1 The Continuous System 121
5-2-2 The NGP Scheme 123
5-2-3 The CIC Scheme 125
5-2-4 Mixed Schemes 127
5-3 The Hierarchy of Charge Assignment Schemes 128
5-3-1 The Long-Range Constraints 129
5-3-2 The Smoothness Constraints 135
5-3-3 The Momentum Conservation Constraint 141
5-3-4 Cloud and Assignment Function Shapes 142
5-4 Truncation Errors 147
5-5 Energy-Conserving Schemes 149
5-6 Transform Space Analysis 152
5-6-1 Charge Assignment 153
5-6-2 The Potential Solver 160
5-6-3 Force Interpolation 162
5-6-4 The Interparticle Force 164

Chapter 6 The Solution of the Field Equations 166

6-1 Introduction 166
6-1-1 Selection of Method 169
6-2 Nonlinear Problems 171
6-2-1 Newton Iteration 171
6-3 Mesh Relaxation 174
6-3-1 Jacobi Method (J) 178
6-3-2 Gauss–Seidel (GS) 178
6-3-3 Successive Overrelaxation (SOR) 179
6-3-4 Chebyshev Acceleration 180
6-3-5 Block Methods 181
6-3-6 Alternating Direction Implicit (ADI) 182
6-4 Matrix Methods 185
6-4-1 Thomas Tridiagonal Algorithm 185
6-4-2 Conjugate-Gradient Algorithm (CGA) 186
6-4-3 Sparse Matrix Methods (SM) 188
6-4-4 Incomplete Decomposition 194
6-4-5 Stone's Strongly Implicit Procedure (SIP) 195
6-4-6 Incomplete-Choleski–Conjugate-Gradient (ICCG) 198
6-5 Rapid Elliptic Solvers (RES) 199
6-5-1 Cyclic Reduction (CR) 201
6-5-2 Multiple Fourier Transform (MFT) 205
6-5-3 FACR Method 208

6-5-4 Convolution Methods 211
6-5-5 James' Algorithm 214
6-5-6 Capacity Matrix Method 215
6-5-7 Concus and Golub Iteration 219
6-6 Concluding Remarks 221

Chapter 7 Collisionless Particle Models 222

7-1 Introduction 222
7-2 The Kinetic Equations 223
7-2-1 Small-Timestep Limit 224
7-2-2 Finite Timestep 225
7-3 The Dispersion Relation 225
7-3-1 Small-Timestep Limit 226
7-3-2 Finite Timestep 229
7-3-3 The Warm-Plasma Approximation 231
7-3-4 Mode Coupling 236
7-4 Finite Multidimensional Systems 241
7-4-1 Periodicity 241
7-4-2 Two and Three Dimensions 242
7-5 Collisions 244
7-6 Conservation Laws 247
7-6-1 Energy 247
7-6-2 Momentum 252
7-6-3 Angular Momentum 253
7-7 Optimization 254
7-7-1 The Interparticle Force 255
7-7-2 One-Dimensional Schemes 256
7-8 Interlacing 260
7-8-1 Force Averaging 262
7-8-2 Harmonic Averaging 264
7-8-3 Multidimensional Schemes 265

Chapter 8 Particle-Particle–Particle-Mesh (P^3M) Algorithms 267

8-1 Introduction 267
8-2 Force Splitting 269
8-3 The Mesh Force 271
8-3-1 Charge Assignment 271
8-3-2 The Force Calculation 272
8-3-3 Errors in the Force 273
8-4 The Short-Range Force 277
8-4-1 The Chaining Mesh 277
8-4-2 The Linked Lists 278
8-4-3 The Momentum Change 279
8-5 The Timing Equation 281

8-6 Optimization 283
8-6-1 Calculation of Force Accuracy 284
8-6-2 Comparison of Schemes 286
8-6-3 The Cost-Quality Relationship 289
8-7 Practical Considerations 292
8-7-1 The Program 293
8-7-2 Data Organization 293
8-7-3 Assignment and Interpolation 295
8-7-4 The Potential Solver 296
8-7-5 The Short-Range Force 299
8-7-6 Parameter Selection 301

Chapter 9 Plasma Simulation 305

9-1 Introduction 305
9-1-1 Magnetohydrodynamics 306
9-1-2 Electrostatic Plasma 308
9-1-3 Historical Survey 309
9-2 Two-Dimensional Electrostatic Model 313
9-2-1 Collision Time 314
9-2-2 Heating Time 316
9-2-3 Empirical Correlations 318
9-3 Anomalous Diffusion 323
9-3-1 Diffusion Experiment 324
9-3-2 Supporting Theory 329
9-3-3 Choice of Timestep and Mesh Size 333
9-3-4 Criticism of the Experiment 337
9-3-5 Two-and-a-Half- and Three-Dimensional Models 338
9-3-6 Diagnostics and Display 339
9-4 The Magnetosphere 342
9-4-1 Magnetohydrodynamic Particle Model 344
9-4-2 Overall Magnetosphere 346
9-4-3 Ampere Particle Model 347
9-4-4 Geomagnetic Tail 351

Chapter 10 Semiconductor Device Simulation 353

10-1 Introduction 353
10-1-1 Purpose of Simulation 353
10-1-2 Defining the Problem 354
10-1-3 Types of Model 358
10-2 Electron Flow in Semiconductors 363
10-2-1 Equations of Motion 363
10-2-2 Band Structure of Gallium Arsenide 367
10-2-3 Scattering Processes 368
10-2-4 Mobility 370
10-2-5 Transient Relaxation Effects 372

10-3 Designing the Computer Model 374
10-3-1 Particle-Mesh Calculation 374
10-3-2 Monte-Carlo Scattering Selection 377
10-3-3 Modified Timestep Cycle 383
10-4 Measurements on FETs 384
10-4-1 Static Characteristics 384
10-4-2 Looking Inside the FET 390
10-4-3 Dynamic Characteristics 393
10-4-4 Lumped-Parameter Equivalent Circuit 397
10-4-5 Noise 400
10-4-6 The COLDFET 405
10-4-7 Complex Geometries 407

Chapter 11 Astrophysics 409

11-1 Introduction 409
11-1-1 Stellar Evolution 409
11-1-2 The Gravitational N-Body Problem 409
11-1-3 Collisional and Collisionless Systems 410
11-1-4 Clustering of Stars and Galaxies 411
11-1-5 The Big Bang 412
11-1-6 Computer Simulation of Stellar Systems 414
11-2 Small Clusters 417
11-2-1 The Force Law 417
11-2-2 Time Integration 418
11-3 Spiral Galaxies 421
11-3-1 Theories of Spiral Structure 421
11-3-2 The Model 422
11-3-3 Choice of Timestep and Mesh Size 424
11-3-4 Collision Time and Particle Number 426
11-3-5 The Ubiquitous Bar Instability 429
11-3-6 Conditions for Spiral Structure 431
11-3-7 The Protogalaxy 438
11-4 Clustering of Galaxies 439
11-4-1 Equations of the Expanding Universe 440
11-4-2 Comoving Coordinates 442
11-4-3 The Simulation Model 444
11-4-4 Results and Conclusions 446

Chapter 12 Solids, Liquids, and Phase Changes 455

12-1 Introduction 455
12-1-1 Molecular Dynamics 455
12-1-2 The Force Law 456
12-1-3 Time Integration 459

12-2 Two-Dimensional Electron Film 460
12-2-1 Dimensionless Equations 460
12-2-2 Choosing the Timestep 461
12-2-3 Scaling the Problem 465
12-2-4 Computer Time and Storage 467
12-2-5 Melting the Electron Film 467
12-3 Ionic Microcrystals 472
12-3-1 Dimensionless Equations 472
12-3-2 Choosing the Timestep 474
12-3-3 Spatial Mesh and Computer Economy 480
12-3-4 Thermodynamic Measurements 481
12-3-5 Measurements in Different Regions 486
12-3-6 Melting, Supercooling, and Glass Formation 488
12-3-7 Radius Ratio, Hardness, and Size Effects 493
12-3-8 Testing Theories of Melting 496

Appendix A Fourier Transforms, Fourier Series, and Finite Fourier Transforms 499

A-1 Transform Definitions 499
A-1-1 The Fourier Transform (FT) 499
A-1-2 The Fourier Series (FS) 501
A-1-3 The Finite Fourier Transform (FFT) 501
A-2 Symmetries 502
A-3 Theorems 502
A-4 Special Functions 505
A-4-1 The "Top-Hat" Function $\Pi(x)$ 505
A-4-2 The "Triangle" Function $\Lambda(x)$ 505
A-4-3 The Gaussian $G(x)$ 505
A-4-4 The Dirac Delta Function $\delta(x)$ 505
A-4-5 The Sampling Function $\text{Ш}(x)$ 506
A-5 Relationship Between Transforms 507
A-6 Multidimensional Transforms 508

Bibliography 509

Index