
Contents

1	Introduction	1
1.1	Why Do We Need Numerical Simulations of Granular Materials?	2
1.2	Organization of the Book	8
1.3	Why Did We Write This Book As Is?	9
2	Molecular Dynamics	13
2.1	Idea of Molecular Dynamics	13
2.1.1	Equations of Motion	13
2.1.2	Boundary Conditions	15
2.1.3	Initial Conditions	16
2.1.4	Models for Spherical Particles	17
2.1.5	Gear's Integration Scheme	26
2.1.6	Sketch of the Molecular Dynamics Algorithm	27
2.1.7	Vector Processing	29
2.2	Overview of the Presented Simulation Programs	30
2.3	Molecular Dynamics Using Spherical Particles	32
2.3.1	Basic Structure and Main Program	32
2.3.2	Simple Algorithm for the Computation of Forces	36
2.3.3	Particle Class Sphere	38
2.3.4	Data Extraction	47
2.3.5	Examples	48
2.3.6	Critical Discussion of the Particle Model	52
2.4	Efficient Force Summation	53
2.4.1	Algorithmic Complexity of the Force Summation	53
2.4.2	Verlet Lists	54
2.4.3	Link Cell Algorithm	61
2.4.4	Lattice Algorithm	65
2.5	Quaternions for Three-Dimensional Simulations	68
2.6	Composite Particles	75
2.6.1	Idea	75

2.6.2	Geometrical Properties	76
2.6.3	Forces	78
2.6.4	Implementation	79
2.6.5	Three-Dimensional Composite Particles	84
2.6.6	Discussion	85
2.7	Simulation of Sharp-Edged Particles	86
2.7.1	Model	86
2.7.2	Interaction of Colliding Triangles	88
2.7.3	Contact Classification	100
2.7.4	Beam Forces	101
2.7.5	Examples	104
2.7.6	Fragmentation of Sharp-Edged Particles	108
2.8	Further Particle Models	108
2.9	Particle Fragmentation	110
2.9.1	Modeling of Fragmentation	110
2.9.2	Molecular Dynamics of Fragmenting Particles	111
2.9.3	Fragmentation Probability	113
2.9.4	Fragment Size Distribution	114
2.10	High Performance Computers	115
2.10.1	Vectorization	116
2.10.2	Parallelization	123
2.11	Vector Class	129
	Program Index	133
3	Event-Driven Molecular Dynamics	135
3.1	Idea and Motivation	135
3.2	Collision of Particles	137
3.3	Uniqueness of the Collision Rule	140
3.4	Sketch of the Algorithm	141
3.5	Coefficients of Restitution	142
3.5.1	Coefficient of Normal Restitution ε^n	142
3.5.2	Tangential Coefficient of Restitution ε^t	144
3.5.3	Relation between ε^n and ε^t	146
3.6	Simple Algorithm	
	for Event-Driven Molecular Dynamics	147
3.6.1	Overview	147
3.6.2	Force-Free Motion of Particles	148
3.6.3	Pairwise Particle Collisions	148
3.6.4	Wall Collisions	151
3.6.5	Initialization	153
3.6.6	Schedule of Collision Times	153
3.6.7	Main Program	155
3.6.8	Output	156
3.6.9	A Note on Numerical Errors	157
3.6.10	Critical Discussion of the Algorithm	160

3.7	Improved Algorithm for Event-Driven Molecular Dynamics	160
3.7.1	Reduction of the Collision List	160
3.7.2	Data Organization	162
3.7.3	Removal of Invalid Entries from the Event Lists	163
3.7.4	Collision-Free Motion of Particles	163
3.7.5	Optimal Box Size	165
3.7.6	Scheduling Events	166
3.7.7	Update of Particle Positions	167
3.7.8	Efficiency of the Algorithm	167
3.8	Boundary Conditions	168
3.8.1	Reflecting Boundaries	169
3.8.2	Periodic Boundary Conditions	170
3.8.3	Heated Walls	173
3.9	Inelastic Collapse	177
3.10	Granular Gases	179
3.10.1	What are Granular Gases?	179
3.10.2	Cluster Instability	180
3.10.3	Some Open Problems	181
	Program Index	189
4	Direct Simulation Monte Carlo	191
4.1	Idea of Direct Simulation Monte Carlo	191
4.2	Boltzmann Equation	193
4.3	Collision Frequency of a Uniform Hard Sphere Gas	197
4.4	Integration of the Boltzmann Equation	198
4.5	Implementation	200
4.6	Application to a Force-Free Granular Gas	206
5	Rigid-Body Dynamics	211
5.1	Rigid Bodies	211
5.2	Sketch of the Algorithm	215
5.3	Mathematical Description	215
5.3.1	Frictionless Particles	215
5.3.2	Particle Systems with Friction	219
5.4	Dantzig's Algorithm for the Computation of the Forces	221
5.4.1	General Scheme	221
5.4.2	Application of the Algorithm to a Simple Example ...	224
5.5	Collisions	232
5.6	Resolution of Static Indeterminacy	236
5.7	Integration of the Equation of Motion	238
5.8	Simple Examples	239
5.9	Discussion of the Model	241

- 6 Cellular Automata** 243
 - 6.1 Overview 243
 - 6.2 Heap Formation and Avalanches 243
 - 6.3 Formation of Ripples 250
 - 6.4 Lattice Gas Simulations 255
 - 6.4.1 Lattice Gas Automaton 255
 - 6.4.2 Granular Pipe Flow 257
 - 6.4.3 Density Inhomogeneities in Granular Pipe Flow 268

- 7 Bottom-to-Top Reconstruction** 271
 - 7.1 Idea of the Method 271
 - 7.2 Simulating a Heap 273
 - 7.3 Dynamic Simulations 287
 - 7.4 Critical Analysis of the Model 290

- 8 Brownian Dynamics for the Simulation of Granular Flows** 293
 - 8.1 Langevin Equation for Pipe Flow 293
 - 8.2 Simulation of the Langevin Equation 296

- References** 303

- Index** 319