

Contents

1	Introduction: Additive/3D Printing Materials—Filaments, Functionalized Inks, and Powders	1
1.1	Objectives	5
	References	6
2	Continuum Methods (CM): Basic Continuum Mechanics	9
2.1	Notation	9
2.2	Kinematics of Deformations	9
2.2.1	Deformation of Line Elements	11
2.3	Equilibrium/Kinetics of Continua	12
2.3.1	Postulates on Volume and Surface Quantities	12
2.3.2	Balance Law Formulations	14
2.4	The First Law of Thermodynamics/An Energy Balance	14
2.5	Linearly Elastic Constitutive Equations	16
2.5.1	The Infinitesimal Strain Case	16
2.5.2	Material Response	16
2.5.3	Material Component Interpretation	18
	References	20
3	CM Approaches: Characterization of Particle-Functionalized Materials	21
3.1	Introduction	21
3.2	Basic Micro–Macro Concepts	22
3.2.1	Testing Procedures	23
3.2.2	The Average Strain Theorem	24
3.2.3	The Average Stress Theorem	25
3.2.4	Satisfaction of Hill’s Energy Condition	25
3.2.5	The Hill–Reuss–Voigt Bounds	26
3.2.6	Improved Estimates	27
	References	28

4	CM Approaches: Estimation and Optimization of the Effective Properties of Mixtures	31
4.1	Combining Bounds	31
4.2	Local Fields: Stresses and Strains	32
4.3	Optimization: Formulation of a Cost Function	34
4.4	Suboptimal Properties Due to Defects—Effects of Pores/voids	40
	References	41
5	CM Approaches: Numerical Thermo-Mechanical Formulations	43
5.1	Transient Thermo-Mechanical Coupled Fields	44
5.2	Iterative Staggering Scheme	46
5.3	Temporal Discretization of Fields	50
5.4	The Overall Solution Scheme	51
5.5	Numerical Examples	54
5.6	Summary and Extensions	59
5.7	Chapter Appendix 1: Summary of Spatial Finite Difference Stencils	62
5.8	Chapter Appendix 2: Second-Order Temporal Discretization	63
5.9	Chapter Appendix 3: Temporally Adaptive Iterative Methods	65
5.10	Chapter Appendix 4: Laser Processing	67
5.10.1	Formulations for Particulate-Laden Continua	68
5.10.2	A Specific Numerical Example—Controlled Heating	69
5.10.3	Numerical Examples	70
5.10.4	Extensions: Advanced Models for Conduction Utilizing Thermal Relaxation	75
	References	78
6	PART II—Discrete Element Method (DEM) Approaches: Dynamic Powder Deposition	83
6.1	Direct Particle Representation/Calculations	86
6.1.1	Comments on Rolling	86
6.1.2	Particle-to-particle Contact Forces	87
6.1.3	Particle-Wall Contact	88
6.1.4	Contact Dissipation	88
6.1.5	Regularized Contact Friction Models	89
6.1.6	Particle-to-particle Bonding Relation	90
6.1.7	Electromagnetic Forces	90
6.1.8	Inter-particle Near-Field Interaction	91
6.1.9	Magnetic Forces	92
6.1.10	Interstitial Damping	92
6.2	Time-Stepping	93

6.2.1	Iterative (Implicit) Solution Method	93
6.2.2	Algorithm	95
6.3	Thermal Fields	97
6.3.1	Heat Transfer Model	97
6.3.2	Lasers—Various Levels of Description	98
6.3.3	Numerical Integration	100
6.4	Total System Coupling: Multiphysical Staggering Scheme	100
6.4.1	A General Iterative Framework	101
6.4.2	Overall Solution Algorithm	101
6.4.3	Interaction Lists	102
6.5	Numerical Examples	104
6.6	Summary for DEM Approaches	108
6.7	Chapter Appendix 1: Contact Area Parameter and Alternative Models	109
6.8	Chapter Appendix 2: Phase Transformations	112
	References	113
7	DEM Extensions: Electrically Driven Deposition of Polydisperse Particulate Powder Mixtures	121
7.1	Introduction	121
7.2	Algorithm	122
7.3	Numerical Examples of Involving Polydisperse Depositions	123
	References	133
8	DEM Extensions: Electrically Aided Compaction and Sintering	135
8.1	Introduction	135
8.1.1	Objectives	135
8.2	Direct Particle Representation	137
8.3	Thermal Fields	138
8.3.1	Governing Equations	138
8.3.2	Numerical Integration	139
8.4	Modeling of Current Flow	140
8.4.1	Particle Model Simplification	140
8.4.2	Iterative Flux Summation/Solution Process	141
8.4.3	Overall Solution Algorithm	143
8.5	Numerical Examples	144
8.5.1	STEP 1: Pouring the Particles	145
8.5.2	STEP 2: Compacting the Particles	145
8.6	Extensions and Conclusions	148
8.7	Chapter Appendix 1: Joule-Heating	149
8.7.1	Characterizing Electrical Losses	149
8.7.2	Joule-Heating	150

8.8	Chapter Appendix 2: Time-Scaling Arguments for $\frac{\partial P}{\partial t} \approx 0$	150
	References	151
9	DEM Extensions: Flexible Substrate Models	155
9.1	Introduction	155
9.2	A Multibody Dynamics Model for the Particles	156
9.2.1	Overall Contributing Forces	156
9.3	Induced Substrate Stresses	157
9.3.1	Individual Particle Contributions—Normal Load	157
9.3.2	Individual Particle Contributions—Tangential Load	158
9.3.3	Superposition of Contributions for the Total Substrate Stresses	159
9.4	Numerical Examples	161
9.5	Summary, Conclusions, and Extensions	165
	References	166
10	DEM Extensions: Higher-Fidelity Laser Modeling	171
10.1	Propagation of Electromagnetic Energy	172
10.1.1	Electromagnetic Wave Propagation	172
10.1.2	Plane Harmonic Wave Fronts	173
10.1.3	Special Case: Natural (Random) Electromagnetic Energy Propagation	174
10.1.4	Beam Decomposition into Rays	174
10.2	Thermal Conversion of Beam (Optical) Losses	180
10.2.1	Algorithmic Details	181
10.3	Phase Transformations: <i>Solid</i> $\Rightarrow$ <i>Liquid</i> $\Rightarrow$ <i>Vapor</i>	182
10.3.1	Optional Time Scaling and Simulation Acceleration	183
10.4	Numerical Examples	185
10.5	Summary and Extensions	190
10.6	Chapter Appendix: Geometrical Ray Theory	192
	References	194
11	DEM Extensions: Acoustical Pre-Processing	197
11.1	Introduction	197
11.2	Dynamic Response of an Agglomeration	200
11.3	Particle-Shock Wave Contact	200
11.3.1	Ray-Tracing: Incidence, Reflection, and Transmission	201
11.3.2	Acoustical-Pulse Computational Algorithm	203
11.3.3	Iterative (Implicit) Solution Method Algorithm	204
11.4	Numerical Example	205

11.5	Closing Statements	208
11.6	Chapter Appendix: Basics of Acoustics	211
	References	214
12	Summary and Closing Remarks	219
	References	222
	Monograph Appendix A: Elementary Notation and Mathematical Operations	225
	Monograph Appendix B—CM Approaches: Effective Electrical Properties of Mixtures	233
	Monograph Appendix C—CM Approaches: Extensions to Multiphase Materials	257
	Monograph Appendix D—Pumping of Fluidized Particle-Laden Materials	267
	Monograph Appendix E—Hybrid DEM-CM Approaches for Particle-Functionalized Fluids	279