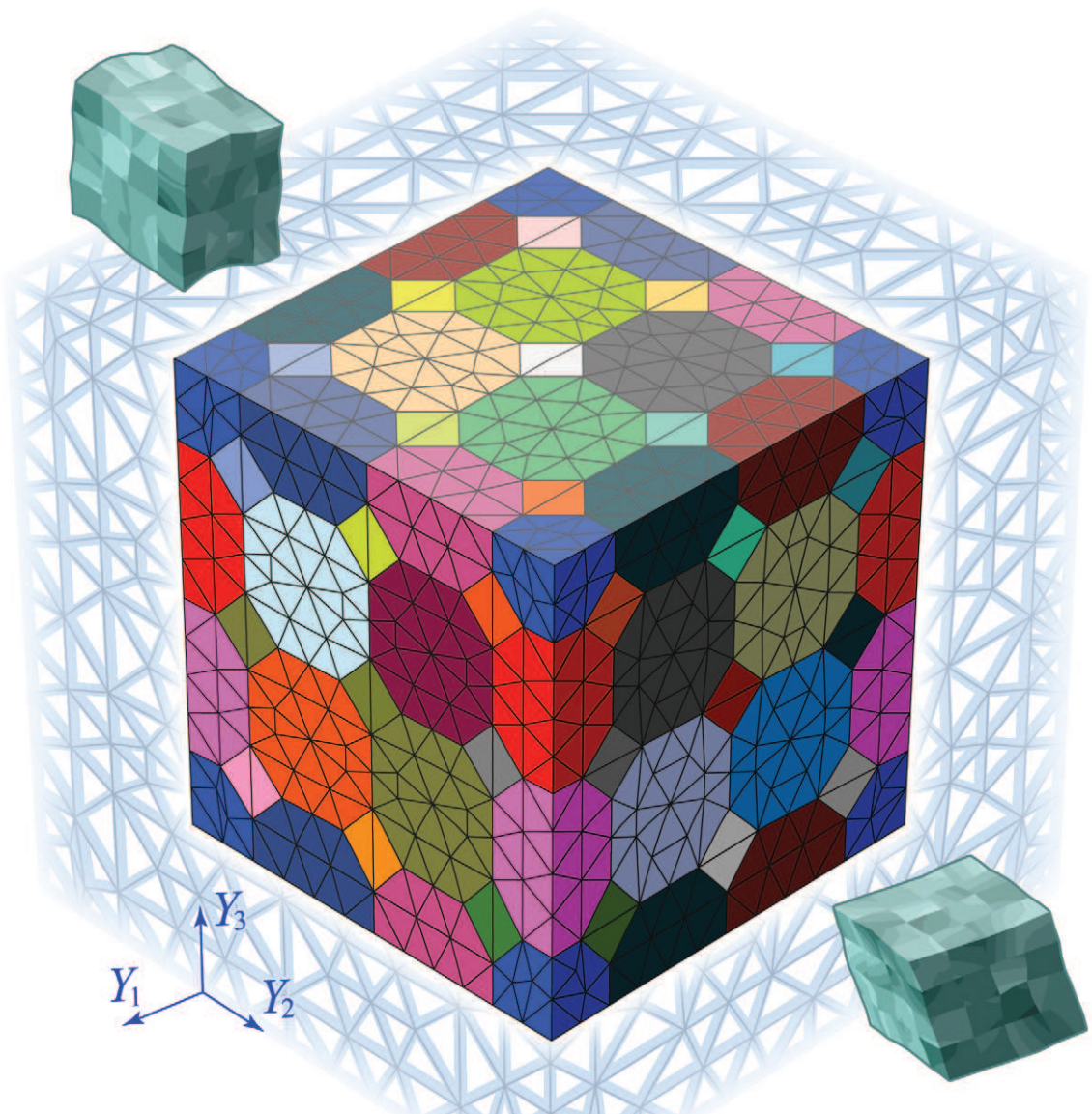


Miguel Vaz Junior, Eduardo A. de Souza  
Neto and Pablo A. Muñoz-Rojas (Eds.)

WILEY-VCH

# Advanced Computational Materials Modeling

From Classical to Multi-Scale Techniques



*Edited by Miguel Vaz Júnior, Eduardo A. de Souza Neto, and  
Pablo A. Muñoz-Rojas*

## **Advanced Computational Materials Modeling**

From Classical to Multi-Scale Techniques



**WILEY-  
VCH**

WILEY-VCH Verlag GmbH & Co. KGaA

## Contents

**Preface** XIII

**List of Contributors** XV

<b>1</b>	<b>Materials Modeling – Challenges and Perspectives</b>	<b>1</b>
	<i>Miguel Vaz Jr., Eduardo A. de Souza Neto, and Pablo Andrés Muñoz-Rojas</i>	
1.1	Introduction	1
1.2	Modeling Challenges and Perspectives	3
1.2.1	Mechanical Degradation and Failure of Ductile Materials	3
1.2.1.1	Remarks	7
1.2.2	Modeling of Cellular Structures	8
1.2.2.1	Remarks	14
1.2.3	Multiscale Constitutive Modeling	15
1.3	Concluding Remarks	18
	Acknowledgments	19
	References	19
<b>2</b>	<b>Local and Nonlocal Modeling of Ductile Damage</b>	<b>23</b>
	<i>José Manuel de Almeida César de Sá, Francisco Manuel Andrade Pires, and Filipe Xavier Costa Andrade</i>	
2.1	Introduction	23
2.2	Continuum Damage Mechanics	25
2.2.1	Basic Concepts of CDM	25
2.2.2	Ductile Plastic Damage	26
2.3	Lemaitre’s Ductile Damage Model	27
2.3.1	Original Model	27
2.3.1.1	The Elastic State Potential	28
2.3.1.2	The Plastic State Potential	29
2.3.1.3	The Dissipation Potential	29
2.3.1.4	Evolution of Internal Variables	30
2.3.2	Principle of Maximum Inelastic Dissipation	31
2.3.3	Assumptions Behind Lemaitre’s Model	32
2.4	Modified Local Damage Models	33
2.4.1	Lemaitre’s Simplified Damage Model	33

2.4.1.1	Constitutive Model	33
2.4.1.2	Numerical Implementation	34
2.4.2	Damage Model with Crack Closure Effect	37
2.4.2.1	Constitutive Model	37
2.4.2.2	Numerical Implementation	40
2.5	Nonlocal Formulations	42
2.5.1	Aspects of Nonlocal Averaging	44
2.5.1.1	The Averaging Operator	44
2.5.1.2	Weight Functions	45
2.5.2	Classical Nonlocal Models of Integral Type	45
2.5.2.1	Nonlocal Formulations for Lemaitre's Simplified Model	46
2.5.3	Numerical Implementation of Nonlocal Integral Models	47
2.5.3.1	Numerical Evaluation of the Averaging Integral	48
2.5.3.2	Global Version of the Elastic Predictor/Return Mapping Algorithm	49
2.6	Numerical Analysis	57
2.6.1	Axisymmetric Analysis of a Notched Specimen	57
2.6.2	Flat Grooved Plate in Plane Strain	62
2.6.3	Upsetting of a Tapered Specimen	63
2.6.3.1	Damage Prediction Using the Lemaitre's Simplified Model	65
2.6.3.2	Damage Prediction Using the Lemaitre's Model with Crack Closure Effect	67
2.7	Concluding Remarks	68
	Acknowledgments	69
	References	69
<b>3</b>	<b>Recent Advances in the Prediction of the Thermal Properties of Metallic Hollow Sphere Structures</b>	<b>73</b>
	<i>Thomas Fiedler, Irina V. Belova, Graeme E. Murch, and Andreas Öchsner</i>	
3.1	Introduction	73
3.2	Methodology	74
3.2.1	Lattice Monte Carlo Method	75
3.2.2	Finite Element Method	77
3.2.2.1	Basics of Heat Transfer	77
3.2.2.2	Weighted Residual Method	77
3.2.2.3	Discretization and Principal Finite Element Equation	78
3.2.3	Numerical Calculation Models	89
3.3	Finite Element Analysis on Regular Structures	91
3.4	Finite Element Analysis on Cubic-Symmetric Models	94
3.5	LMC Analysis of Models of Cross Sections	98
3.5.1	Modeling	98
3.5.2	Results	101
3.6	Computed Tomography Reconstructions	103
3.6.1	Computed Tomography	104
3.6.2	Numerical Analysis	104
3.6.2.1	Microstructure	105

3.6.2.2	Mesostructure	106
3.6.3	Results	106
3.7	Conclusions	108
	References	109
<b>4</b>	<b>Computational Homogenization for Localization and Damage</b>	<b>111</b>
	<i>Thierry J. Massart, Varvara Kouznetsova, Ron H. J. Peerlings, and Marc G. D. Geers</i>	
4.1	Introduction	111
4.1.1	Mechanics Across the Scales	111
4.1.2	Some Historical Notes on Homogenization	112
4.1.3	Separation of Scales	113
4.1.4	Computational Homogenization and Its Application to Damage and Fracture	114
4.2	Continuous–Continuous Scale Transitions	115
4.2.1	First-Order Computational Homogenization	115
4.2.2	Second-Order Computational Homogenization	119
4.2.3	Application of the Continuous–Continuous Homogenization Schemes to Ductile Damage	121
4.3	Continuous–Discontinuous Scale Transitions	125
4.3.1	Scale Transitions and RVE for Initially Periodic Materials	126
4.3.1.1	First-Order Scale Transitions	126
4.3.1.2	Choice of the Mesoscopic Representative Volume Element	127
4.3.1.3	Boundary Conditions for the Unit Cell	128
4.3.2	Localization of Damage at the Fine and Coarse Scales	129
4.3.2.1	Fine-Scale Localization – Implicit Gradient Damage	129
4.3.2.2	Detection of Coarse-Scale Localization as a Bifurcation into an Inhomogeneous Deformation Pattern	130
4.3.2.3	Illustration of the Localization Analysis	132
4.3.2.4	Identification and Selection of the Localization Orientation	135
4.3.3	Localization Band Enhanced Multiscale Solution Scheme	135
4.3.3.1	Introduction of the Localization Band	136
4.3.3.2	Coupled Multiscale Scheme for Localization	137
4.3.4	Scale Transition Procedure for Localized Behavior	139
4.3.4.1	Multiscale Solution Procedure	139
4.3.4.2	Causes of Snapback in the Averaged Material Response	139
4.3.4.3	Strain Jump Control for Embedded Band Snapback	140
4.3.4.4	Dissipation Control for Unit-Cell Snapback	141
4.3.5	Solution Strategy and Computational Aspects	142
4.3.5.1	Governing Equations for the Macroscopic and Mesoscopic Solution Procedures	142
4.3.5.2	Extraction of Consistent Tangent Stiffness for Unit-Cell Snapback Control	144
4.3.5.3	Discretization and Linearization of the Macroscopic Solution Procedure	144

4.3.5.4	Introduction of Localization Bands upon Material Bifurcation	146
4.3.6	Applications and Discussion	147
4.3.6.1	Selection of Localized Solutions	147
4.3.6.2	Mesostructural Snapback in a Tension–Compression Test	149
4.3.6.3	Size Effect in a Shear–Compression Test	151
4.3.6.4	Masonry Shear Wall Test	152
4.4	Closing Remarks	159
	References	160
<b>5</b>	<b>A Mixed Optimization Approach for Parameter Identification Applied to the Gurson Damage Model</b>	<b>165</b>
	<i>Pablo Andrés Muñoz-Rojas, Luiz Antonio B. da Cunda, Eduardo L. Cardoso, Miguel Vaz Jr., and Guillermo Juan Creus</i>	
5.1	Introduction	165
5.2	Gurson Damage Model	166
5.2.1	Influence of the Parameter Values on Behavior of the Damage Model	171
5.2.2	Recent Developments and New Trends in the Gurson Model	175
5.3	Parameter Identification	177
5.4	Optimization Methods – Genetic Algorithms and Mathematical Programming	179
5.4.1	Genetic Algorithms	180
5.4.1.1	Formulation	181
5.4.1.2	Implementation	184
5.4.2	Gradient-Based Methods	184
5.4.2.1	General Procedure	184
5.4.2.2	Sequential Linear Programming (SLP)	185
5.4.2.3	Globally Convergent Method of Moving Asymptotes (GCMMA)	185
5.5	Sensitivity Analysis	187
5.5.1	Modified Finite Differences and the Semianalytical Method	188
5.6	A Mixed Optimization Approach	192
5.7	Examples of Application	192
5.7.1	Low Carbon Steel at 25 °C	192
5.7.2	Aluminum Alloy at 400 °C	197
5.8	Concluding Remarks	200
	Acknowledgments	200
	References	201
<b>6</b>	<b>Semisolid Metallic Alloys Constitutive Modeling for the Simulation of Thixoforming Processes</b>	<b>205</b>
	<i>Roxane Koeune and Jean-Philippe Ponthot</i>	
6.1	Introduction	205
6.2	Semisolid Metallic Alloys Forming Processes	207
6.2.1	Thixotropic Semisolid Metallic Alloys	208
6.2.2	Different Types of Semisolid Processing	209

6.2.2.1	Production of Spheroidal Microstructure	210
6.2.2.2	Reheating	212
6.2.2.3	Forming	213
6.2.3	Advantages and Disadvantages of Semisolid Processing	215
6.3	Rheological Aspects	216
6.3.1	Microscopic Point of View	216
6.3.1.1	Origins of Thixotropy	216
6.3.1.2	Transient Behavior	217
6.3.1.3	Effective Liquid Fraction	222
6.3.2	Macroscopic Point of View	222
6.3.2.1	Temperature Effects	222
6.3.2.2	Yield Stress	222
6.3.2.3	Macrosegregation	223
6.4	Numerical Background in Large Deformations	223
6.4.1	Kinematics in Large Deformations	223
6.4.1.1	Lagrangian Versus Eulerian Coordinate Systems	223
6.4.1.2	Deformation Gradient and Strain Rate Tensors	225
6.4.2	Finite Deformation Constitutive Theory	225
6.4.2.1	Principle of Objectivity	225
6.4.2.2	Different Classes of Materials	226
6.4.2.3	A Corotational Formulation	228
6.4.2.4	Linear Elastic Solid Material Model	229
6.4.2.5	Linear Newtonian Liquid Material Model	230
6.4.2.6	Hypoelastic Solid Material Models	231
6.4.2.7	Liquid Material Models	236
6.4.2.8	Comparison of Solid and Liquid Approaches	236
6.5	State-of-the-Art in FE-Modeling of Thixotropy	237
6.5.1	One-Phase Models	237
6.5.1.1	Apparent Viscosity Evolution	238
6.5.1.2	Yield Stress Evolution	243
6.5.2	Two-Phase Models	244
6.5.2.1	Two Coupled Fields	244
6.5.2.2	Coupling Sources	245
6.6	A Detailed One-Phase Model	246
6.6.1	Cohesion Degree	247
6.6.2	Liquid Fraction	248
6.6.3	Viscosity Law	248
6.6.4	Yield Stress and Isotropic Hardening	250
6.7	Numerical Applications	250
6.7.1	Test Description	250
6.7.2	Results Analysis	251
6.7.2.1	First Validation of the Model under Isothermal Conditions	251
6.7.2.2	Thermomechanical Analysis	252
6.7.2.3	Residual Stresses Analysis	253
6.7.2.4	Internal Variables Analysis	253

6.8	Conclusion	254
	References	255
<b>7</b>	<b>Modeling of Powder Forming Processes; Application of a Three-invariant Cap Plasticity and an Enriched Arbitrary Lagrangian–Eulerian FE Method</b>	<b>257</b>
	<i>Amir R. Khoei</i>	
7.1	Introduction	257
7.2	Three-Invariant Cap Plasticity	260
7.2.1	Isotropic and Kinematic Material Functions	262
7.2.2	Computation of Powder Property Matrix	264
7.2.3	Model Assessment and Parameter Determination	265
7.2.3.1	Model Assessment	265
7.2.3.2	Parameter Determination	267
7.3	Arbitrary Lagrangian–Eulerian Formulation	269
7.3.1	ALE Governing Equations	270
7.3.2	Weak Form of ALE Equations	272
7.3.3	ALE Finite Element Discretization	273
7.3.4	Uncoupled ALE Solution	274
7.3.4.1	Material (Lagrangian) Phase	275
7.3.4.2	Smoothing Phase	276
7.3.4.3	Convection (Eulerian) Phase	278
7.3.5	Numerical Modeling of an Automotive Component	279
7.4	Enriched ALE Finite Element Method	282
7.4.1	The Extended-FEM Formulation	283
7.4.2	An Enriched ALE Finite Element Method	286
7.4.2.1	Level Set Update	287
7.4.2.2	Stress Update and Numerical Integration	288
7.4.3	Numerical Modeling of the Coining Test	291
7.5	Conclusion	295
	Acknowledgments	295
	References	296
<b>8</b>	<b>Functionally Graded Piezoelectric Material Systems – A Multiphysics Perspective</b>	<b>301</b>
	<i>Wilfredo Montealegre Rubio, Sandro Luis Vatanabe, Gláucio Hermogenes Paulino, and Emilio Carlos Nelli Silva</i>	
8.1	Introduction	301
8.2	Piezoelectricity	302
8.3	Functionally Graded Piezoelectric Materials	304
8.3.1	Functionally Graded Materials (FGMs)	304
8.3.2	FGM Concept Applied to Piezoelectric Materials	306
8.4	Finite Element Method for Piezoelectric Structures	309
8.4.1	The Variational Formulation for Piezoelectric Problems	309
8.4.2	The Finite Element Formulation for Piezoelectric Problems	310



8.4.3	Modeling Graded Piezoelectric Structures by Using the FEM	312
8.5	Influence of Property Scale in Piezotransducer Performance	314
8.5.1	Graded Piezotransducers in Ultrasonic Applications	314
8.5.2	Further Consideration of the Influence of Property Scale: Optimal Material Gradation Functions	319
8.6	Influence of Microscale	322
8.6.1	Performance Characteristics of Piezocomposite Materials	326
8.6.1.1	Low-Frequency Applications	326
8.6.1.2	High-Frequency Applications	328
8.6.2	Homogenization Method	328
8.6.3	Examples	332
8.7	Conclusion	335
	Acknowledgments	335
	References	336
<b>9</b>	<b>Variational Foundations of Large Strain Multiscale Solid Constitutive Models: Kinematical Formulation</b>	<b>341</b>
	<i>Eduardo A. de Souza Neto and Raúl A. Feijóo</i>	
9.1	Introduction	341
9.2	Large Strain Multiscale Constitutive Theory: Axiomatic Structure	343
9.2.1	Deformation Gradient Averaging and RVE Kinematics	346
9.2.1.1	Consequence: Minimum RVE Kinematical Constraints	346
9.2.1.2	Minimum Constraint on Displacement Fluctuations	347
9.2.2	Actual Constraints: Spaces of RVE Velocities and Virtual Displacements	348
9.2.3	Equilibrium of the RVE	349
9.2.3.1	Strong Form of Equilibrium	350
9.2.3.2	Solid–Void/Pore Interaction	350
9.2.4	Stress Averaging Relation	351
9.2.4.1	Macroscopic Stress in Terms of RVE Boundary Tractions and Body Forces	351
9.2.5	The Hill–Mandel Principle of Macrohomogeneity	352
9.3	The Multiscale Model Definition	353
9.3.1	The Microscopic Equilibrium Problem	354
9.3.2	The Multiscale Model: Well-Posed Equilibrium Problem	354
9.4	Specific Classes of Multiscale Models: The Choice of $\mathcal{V}_\mu$	356
9.4.1	Taylor Model	356
9.4.1.1	The Taylor-Based Constitutive Functional: the Rule of Mixtures	357
9.4.2	Linear RVE Boundary Displacement Model	359
9.4.3	Periodic Boundary Displacement Fluctuations Model	359
9.4.4	Minimum Kinematical Constraint: Uniform Boundary Traction	360
9.5	Models with Stress Averaging in the Deformed RVE Configuration	361
9.6	Problem Linearization: The Constitutive Tangent Operator	362
9.6.1	Homogenized Constitutive Functional	363
9.6.2	The Homogenized Tangent Constitutive Operator	364

9.7	Time-Discrete Multiscale Models	366
9.7.1	The Incremental Equilibrium Problem	367
9.7.2	The Homogenized Incremental Constitutive Function	367
9.7.3	Time-Discrete Homogenized Constitutive Tangent	368
9.7.3.1	Taylor Model	369
9.7.3.2	The General Case	369
9.8	The Infinitesimal Strain Theory	371
9.9	Concluding Remarks	372
	Appendix	373
	Acknowledgments	376
	References	376
<b>10</b>	<b>A Homogenization-Based Prediction Method of Macroscopic Yield Strength of Polycrystalline Metals Subjected to Cold-Working</b>	<b>379</b>
	<i>Kenjiro Terada, Ikumu Watanabe, Masayoshi Akiyama, Shigemitsu Kimura, and Kouichi Kuroda</i>	
10.1	Introduction	379
10.2	Two-Scale Modeling and Analysis Based on Homogenization Theory	382
10.2.1	Two-Scale Boundary Value Problem	383
10.2.2	Micro–Macro Coupling and Decoupling Schemes for the Two-Scale BVP	385
10.2.3	Method of Evaluating Macroscopic Yield Strength after Cold-Working	386
10.3	Numerical Specimens: Unit Cell Models with Crystal Plasticity	387
10.4	Approximate Macroscopic Constitutive Models	390
10.4.1	Definition of Macroscopic Yield Strength	391
10.4.2	Macroscopic Yield Strength at the Initial State	391
10.4.3	Approximate Macroscopic Constitutive Model	393
10.4.4	Parameter Identification for Approximate Macroscopic Constitutive Model	393
10.5	Macroscopic Yield Strength after Three-Step Plastic Forming	395
10.5.1	Forming Condition	395
10.5.2	Two-Scale Analyses with Micro–Macro Coupling and Decoupling Schemes	396
10.5.3	Evaluation of Macroscopic Yield Strength after Three-Step Plastic Forming	398
10.6	Application for Pilger Rolling of Steel Pipe	401
10.6.1	Forming Condition	401
10.6.2	Decoupled Microscale Analysis	403
10.6.3	Evaluation of Macroscopic Yield Strength after Pilger Rolling Process	406
10.7	Conclusion	408
	References	409
	<b>Index</b>	<b>413</b>

## Preface

The systematic analysis of solid mechanics problems using numerical techniques can be traced back to the 1960s and 1970s following the development of the finite element method. The early approaches to elastic materials and, to a certain extent, inelastic problems, paved the way to an all-encompassing discipline known today as *computational materials modelling*.

As computer technologies have evolved, placing portable computers on the desk of virtually every university staff and graduate student, numerical techniques and algorithms have experienced extraordinary advances in a wide range of engineering fields. The development of new computational modelling strategies, especially those based on the finite element method, has prompted new applications such as crystal plasticity, damage and multi-scale formulations, semi-solid, particulate, porous and functionally graded materials amongst others.

This book was conceived in an attempt to congregate innovative modelling approaches so that graduate students and researchers, both from academia and industry, can use it as a springboard to further advancements. It is also important to say that this book is by no means exhaustive on the subject of materials modelling and some advanced readers would probably have appreciated the inclusion of further details on the underlying mathematical formulations. For the sake of objectivity, we have focussed on topics which show not only new and innovative modelling strategies, but also on sound physical foundations and both promising and direct application to engineering problems. Emphasis is placed on computational modelling rather than materials processing, although illustrative examples featuring some process applications are also included. A review of the state-of-the-art modelling approaches as well as a discussion on future trends and advancements is also presented by the contributors.

Finally we would like to sincerely thank all the authors for their time and commitment to produce such high quality chapters. We really appreciate their contribution.

July 2010

*Miguel Vaz Jr.*  
*Eduardo A. de Souza Neto*  
*Pablo A. Muñoz-Rojas*

## List of Contributors

### **Masayoshi Akiyama**

Kyoto Institute of Technology  
Department of Mechanical  
Engineering  
Gosho-Kaido-cho  
Matsugasaki  
Sakyo-ku  
Kyoto 606-8585  
Japan

### **Filipe Xavier Costa Andrade**

University of Porto  
Faculty of Engineering  
Rua Dr. Roberto Frias  
4200-465 Porto  
Portugal

### **Irina V. Belova**

University of Newcastle  
University Centre for Mass and  
Thermal Transport in  
Engineering Materials  
Priority Research Centre for  
Geotechnical and Materials  
Modelling  
School of Engineering  
Callaghan, NSW 2308  
Australia

### **Eduardo L. Cardoso**

State University of  
Santa Catarina  
Department of Mechanical  
Engineering Centre for  
Technological Sciences  
Campus Universitário Prof.  
Avelino Marcante  
Santa Catarina  
89223-100 – Joinville  
Brazil

### **José Manuel de Almeida**

**César de Sá**  
University of Porto  
Faculty of Engineering  
Rua Dr. Roberto Frias  
4200-465 Porto  
Portugal

### **Guillermo Juan Creus**

Federal University of  
Rio Grande do Sul  
Department of Civil Engineering  
Centre for Computational and  
Applied Mechanics  
Rua Osvaldo Aranha  
90035-190 – Porto Alegre  
99, Rio Grande do Sul  
Brazil

**Luiz Antonio B. da Cunda**

Federal University of Rio Grande Foundation  
School of Engineering  
Rua Alfredo Huch  
96201-900 – Rio Grande  
475, Rio Grande do Sul  
Brazil

**Raúl A. Feijóo**

Laboratório Nacional de Computação Científica (LNCC/MCT) & Instituto Nacional de Ciência e Tecnologia em Medicina Assistida por Computação Científica (INCT-MACC) Av. Getúlio Vargas 333  
Quitandinha  
CEP 25651-070  
Petrópolis – RJ  
Brazil

**Thomas Fiedler**

University of Newcastle  
University Centre for Mass and Thermal Transport in Engineering Materials  
Priority Research Centre for Geotechnical and Materials Modelling  
School of Engineering  
Callaghan, NSW 2308  
Australia

**Marc G. D. Geers**

Eindhoven University of Technology  
Department of Mechanical Engineering  
P.O. Box 513  
5600 MB Eindhoven  
Netherlands

**Amir R. Khoei**

Sharif University of Technology  
Department of Civil Engineering  
Center of Excellence in Structures and Earthquake Engineering  
P.O. Box. 11365-9313  
Tehran  
Iran

**Shigemitsu Kimura**

Pipe & Tube Company  
Sumitomo Metal Industries Ltd.  
1 Higashi-mukoujima  
Amagasaki  
Hyogo 660-0856  
Japan

**Roxane Koeune**

University of Liège  
Aerospace and Mechanical Engineering Department  
1 Chemin des Chevreuils  
B4000 Liège  
Belgium

**Varvara Kouznetsova**

Eindhoven University of Technology  
Department of Mechanical Engineering  
P.O. Box 513  
5600 MB  
Eindhoven  
Netherlands

**Kouichi Kuroda**

Corporate R & D Laboratories  
Sumitomo Metal Industries Ltd.  
1-8 Fuso-cho, Amagasaki  
Hyogo 660-0891  
Japan

**Thierry J. Massart**

Université Libre de  
Bruxelles (ULB)  
Building Architecture  
and Town Planning  
CP 194/2  
Av. F.-D. Roosevelt 50  
1050 Brussels  
Belgium

**Pablo Andrés Muñoz-Rojas**

Santa Catarina State  
University - UDESC  
Department of Mechanical  
Engineering  
Centre for Technological Sciences  
Campus Universitário Prof.  
Avelino Marcante  
89223-100, Joinville  
Santa Catarina  
Brazil

**Graeme E. Murch**

University of Newcastle  
University Centre for Mass and  
Thermal Transport in  
Engineering Materials  
Priority Research Centre for  
Geotechnical and Materials  
Modelling  
School of Engineering  
Callaghan, NSW 2308  
Australia

**Eduardo A. de Souza Neto**

Swansea University  
Civil and Computational  
Engineering Centre  
School of Engineering  
Singleton Park  
SA2 8PP  
Swansea  
UK

**Gláucio Hermogenes Paulino**

University of Illinois at  
Urbana-Champaign  
Newmark Laboratory  
Department of Civil and  
Environment Engineering  
205 North Mathews Av.  
Urbana  
IL 61801  
USA

**Ron H. J. Peerlings**

Eindhoven University of  
Technology  
Department of Mechanical  
Engineering  
P.O. Box 513  
5600 MB Eindhoven  
Netherlands

**Francisco Manuel Andrade Pires**

University of Porto  
Faculty of Engineering  
Rua Dr. Roberto Frias  
4200-465 Porto  
Portugal

**Jean-Philippe Ponthot**

University of Liège  
Aerospace and Mechanical  
Engineering Department  
1 Chemin des Chevreuils  
B4000 Liège  
Belgium

**Wilfredo Montealegre Rubio**

National University of Colombia  
School of Mechatronic of  
the Faculty of Mine  
Carrera 80 No. 65-223  
bloque M8, oficina 113  
Medellin, Antioquia  
Colombia

**Emílio Carlos Nelli Silva**

University of São Paulo  
Department of Mechatronics and  
Mechanical Systems Engineering  
Av. Prof. Mello Moraes  
2231 - Cidade Universitária  
São Paulo  
05508-900  
Brazil

**Kenjiro Terada**

Tohoku University  
Department of  
Civil Engineering  
Aza-Aoba 6-6-06  
Aramaki  
Aoba-ku  
Sendai 980-8579  
Japan

**Sandro Luis Vatanabe**

University of São Paulo  
Department of Mechatronics and  
Mechanical Systems Engineering  
Av. Prof. Mello Moraes  
2231 - Cidade Universitária  
São Paulo  
05508-900  
Brazil

**Miguel Vaz Jr.**

Santa Catarina State  
University - UDESC  
Department of Mechanical  
Engineering  
Centre for Technological Sciences  
Campus Universitário Prof.  
Avelino Marcante  
89223-100 Joinville  
Santa Catarina  
Brazil

**Ikumu Watanabe**

National Institute for  
Materials Science  
Structural Metals Center  
Sengen 1-2-1  
Tsukuba  
Ibaraki 305-0047  
Japan

**Andreas Öchsner**

Technical University of Malaysia  
Department of Applied  
Mechanics  
Faculty of Mechanical  
Engineering  
Skudai  
Johor  
81310 UTM  
Malaysia

*and*

University of Newcastle  
University Centre for Mass and  
Thermal Transport in  
Engineering Materials  
Priority Research Centre for  
Geotechnical and Materials  
Modelling  
School of Engineering  
Callaghan, NSW 2308  
Australia

## 7

## Modeling of Powder Forming Processes; Application of a Three-invariant Cap Plasticity and an Enriched Arbitrary Lagrangian–Eulerian FE Method

Amir R. Khoei

## 7.1

### Introduction

Powder metallurgy is a highly developed method of manufacturing reliable ferrous and nonferrous parts. The powder metallurgy process is cost-effective, because it minimizes machining, produces good surface finish, and maintains close dimensional tolerances. The method is a material-processing technique utilized to achieve a coherent near-to-net shape industrial component. The often extremely high tolerance requirements of the parts and the cost for hard machining of a sintered component are a challenge for die pressing. One of the main difficulties that exists in the compaction-forming process of powders includes a nonhomogeneous density distribution, which has wide ranging effects on the final performance of the compacted part. The variation of density results in cracks and also in localized deformation in the compact, producing regions of high density surrounded by lower density material, leading to compact failure. The lack of homogeneity is primarily caused by friction, due to interparticle movement, as well as relative slip between powder particles and the die wall. The die geometry and the sequence of movement result in a lack of homogeneity of density distribution in a compact. Thus, the success of compaction forming depends on the ability of the process in imparting a uniform density distribution in the engineered part. In order to perform such analysis, the complex mechanisms of compaction process must be drawn into a mathematical formulation with the knowledge of material behavior.

A number of constitutive models have been developed for the compaction of powders over the last three decades, including micromechanical models [1–3], flow formulations [4], and solid mechanics models [5–11]. The porous material model, generally known as a *modified von Mises criterion* [12], has been used for the simulation of powder-forming processes. This model includes the influence of the hydrostatic stress component, and satisfies the symmetry and convexity conditions required for the development of a plasticity theory. The yielding of porous materials is more complicated than that of fully dense materials, because the onset of yielding is influenced not only by the deviatoric stress components