

CONTENTS

Preface	xi
I Foundations	1
1 Introduction	3
2 Basic Concepts of Artificial Chemistries	11
2.1 Modeling and Simulation	11
2.2 Chemistry Concepts	15
2.3 General Structure of an Artificial Chemistry	25
2.4 A Few Important Distinctions	31
2.5 Two Examples	33
2.6 Frequently Used Techniques in ACs	38
2.7 Summary	43
3 The Matrix Chemistry as an Example	45
3.1 The Basic Matrix Chemistry	46
3.2 The Simplest System, $N = 4$	50
3.3 The System $N = 9$	55
3.4 Systems with Larger N	59
3.5 Summary	61
4 Computing Chemical Reactions	63
4.1 From Macroscopic to Microscopic Chemical Dynamics	63
4.2 Stochastic Reaction Algorithms	65
4.3 Spatial and Multicompartmental Algorithms	71
4.4 Summary	73
Life and Evolution	75
5 The Chemistry of Life	77
5.1 What Is Life?	79
5.2 The Building Blocks of Life	80
5.3 The Organization of Modern Cells	93
5.4 Multicellular Organisms	100
5.5 Summary	109

6 The Essence of Life	111
6.1 A Minimal Cell	111
6.2 Origin of Life	119
6.3 Artificial Chemistry Contributions to Origin of Life Research	130
6.4 Summary	136
7 Evolution	139
7.1 Evolution: Taming Combinatorics to Improve Life	140
7.2 Evolutionary Dynamics from an AC Perspective	141
7.3 Artificial Chemistries for Evolution	154
7.4 Summary and Open Issues	157
8 Complexity and Open-Ended Evolution	159
8.1 Evolution: Steering Self-Organization and Promoting Innovation	159
8.2 Coevolutionary Dynamics in Ecologies	161
8.3 Robustness and Evolvability	165
8.4 Complexity Growth	169
8.5 Toward Open-Ended Artificial Evolution	175
8.6 Summary	177
III Approaches to Artificial Chemistries	179
9 Rewriting Systems	181
9.1 Lambda Calculus	182
9.2 Gamma	184
9.3 The Chemical Abstract Machine	186
9.4 Chemical Rewriting System on Multisets	187
9.5 P systems	188
9.6 MGS	191
9.7 Other Formal Calculi Inspired by a Chemical Metaphor	193
9.8 L-Systems and Other Rewriting Systems	193
9.9 Summary	194
10 Automata and Machines	195
10.1 Finite State Automata	196
10.2 Turing Machines	197
10.3 Von Neumann Machines	198
10.4 Cellular Automata	200
10.5 Examples of Artificial Chemistries Based on Turing Machines	202
10.6 Artificial Chemistries Based on von Neumann Machines	207
10.7 Artificial Chemistries Based on Cellular Automata	215
10.8 Summary	222
11 Bio-Inspired Artificial Chemistries	225
11.1 String-Based Artificial Chemistries	225
11.2 Lock-and-Key Artificial Chemistries	234
11.3 Networks	240
11.4 Spatial Structuring and Movement in Artificial Chemistries	248
11.5 Summary	254

IV Order Construction	255
12 The Structure of Organizations	257
12.1 Basic Definitions	259
12.2 Generators	262
12.3 Bringing Order into Organizations	263
12.4 Novelty and Innovation	265
12.5 Examples of the Statics of Organizations	266
12.6 How to Calculate Closed and Self-Maintaining Sets	270
12.7 Summary	273
13 The Dynamics of Organizations	275
13.1 Flows, Stoichiometry and Kinetic Constants	275
13.2 Examples of the Dynamics of Organization	277
13.3 Observing Organizations	282
13.4 Probabilistic Notions of Closure and Self-Maintenance	283
13.5 Summary	285
14 Self-Organization and Emergent Phenomena	287
14.1 Examples of Self-Organizing Systems	288
14.2 Explanatory Concepts of Self-Organization	289
14.3 The Emergence of Phenomena	295
14.4 Explanatory Concepts of Emergence	298
14.5 Emergence and Top-Down Causation	304
14.6 Summary	306
15 Constructive Dynamical Systems	307
15.1 Novelty, Innovation, Emergence	307
15.2 Birth Processes at the Same Level	309
15.3 The Emergence of Entities on a Higher Level	317
15.4 Summary	319
V Applications	321
16 Applications of Artificial Chemistries	323
16.1 Robots Controlled by Artificial Chemistries	324
16.2 ACs for Networking	330
16.3 Language Dynamics and Evolution	334
16.4 Music Composition Using Algorithmic Chemistries	338
16.5 Proof Systems	339
16.6 Artificial Chemistry and Genetic Programming	340
16.7 Summary	344
17 Computing with Artificial Chemistries	345
17.1 Principles of implementation	346
17.2 Search and Optimization Algorithms Inspired by Chemistry	355
17.3 Distributed Algorithms Using Chemical Computing	358
17.4 <i>In Silico</i> Simulation of Wet Chemical Computing	366
17.5 Summary	372

18 Modeling Biological Systems	373
18.1 Folding Algorithms	374
18.2 Basic Kinetics of Biomolecular Interactions	379
18.3 Biochemical Pathways	383
18.4 Modeling Genetic Regulatory Networks	391
18.5 Cell Differentiation and Multicellularity	396
18.6 Morphogenesis	398
18.7 Summary	403
19 Wet Artificial Chemistries	405
19.1 Artificial Building Blocks of Life	405
19.2 Synthetic Life and Protocells	411
19.3 Chemical and Biochemical Computation	417
19.4 <i>In Vivo</i> Computing with Bacteria and Other Living Organisms	431
19.5 Ethical Issues	435
19.6 Summary	437
20 Beyond Chemistry and Biology	439
20.1 Mechanical Self-Assembly	439
20.2 Nuclear and Particle Physics	442
20.3 Economic Systems	444
20.4 Social Systems	446
20.5 Summary	448
VI Conclusions	449
21 Summary and Perspectives	451
21.1 Some Common Criticisms of the Artificial Chemistry Approach	451
21.2 Delimiting the Borders of the Field	453
21.3 Main Features of Artificial Chemistries	456
21.4 Conclusion	459
Further Reading	461
Appendix: Setting up Your Own Artificial Chemistry System	465
The PyCellChemistry Package	465
Writing Your Own Artificial Chemistry in Python	468
Further Resources	478
Bibliography	481
Author Index	531
Subject Index	545