PREFACE

The field of Artificial Life (ALife) is now firmly established in the scientific world. A number of conference series have been founded, books and edited volumes have been written, journals are being published, and software has taken up the philosophy of Artificial Life. One of the original goals of the field of Artificial Life, the understanding of the emergence of life on Earth, however, has not (yet) been achieved. It has been argued that, before life could emerge on the planet, more primitive forms of self-organization might have been necessary. So just as life likely was preceded by a prebiotic phase of the organization of macromolecules, perhaps Artificial Life would gain from the introduction of models explicitly studying chemical reaction systems. It is from this motivation that artificial chemistries were conceived.

Artificial chemistries (ACs) have been around for more than two decades. Perhaps sometimes in disguise, they have been a fascinating topic for scientist of numerous disciplines, mathematicians and computer scientists foremost among them. From the term itself we can glean that they are not primarily meant to produce new materials, but rather new interactions. The interactions between molecules are to be man-made, and the molecules themselves might be artificial, or even virtual. As a consequence, the results of artificial chemistries can be found in the virtual world, e.g. in certain multiagent systems, or in the real world, in the form of new (artificial) reaction systems.

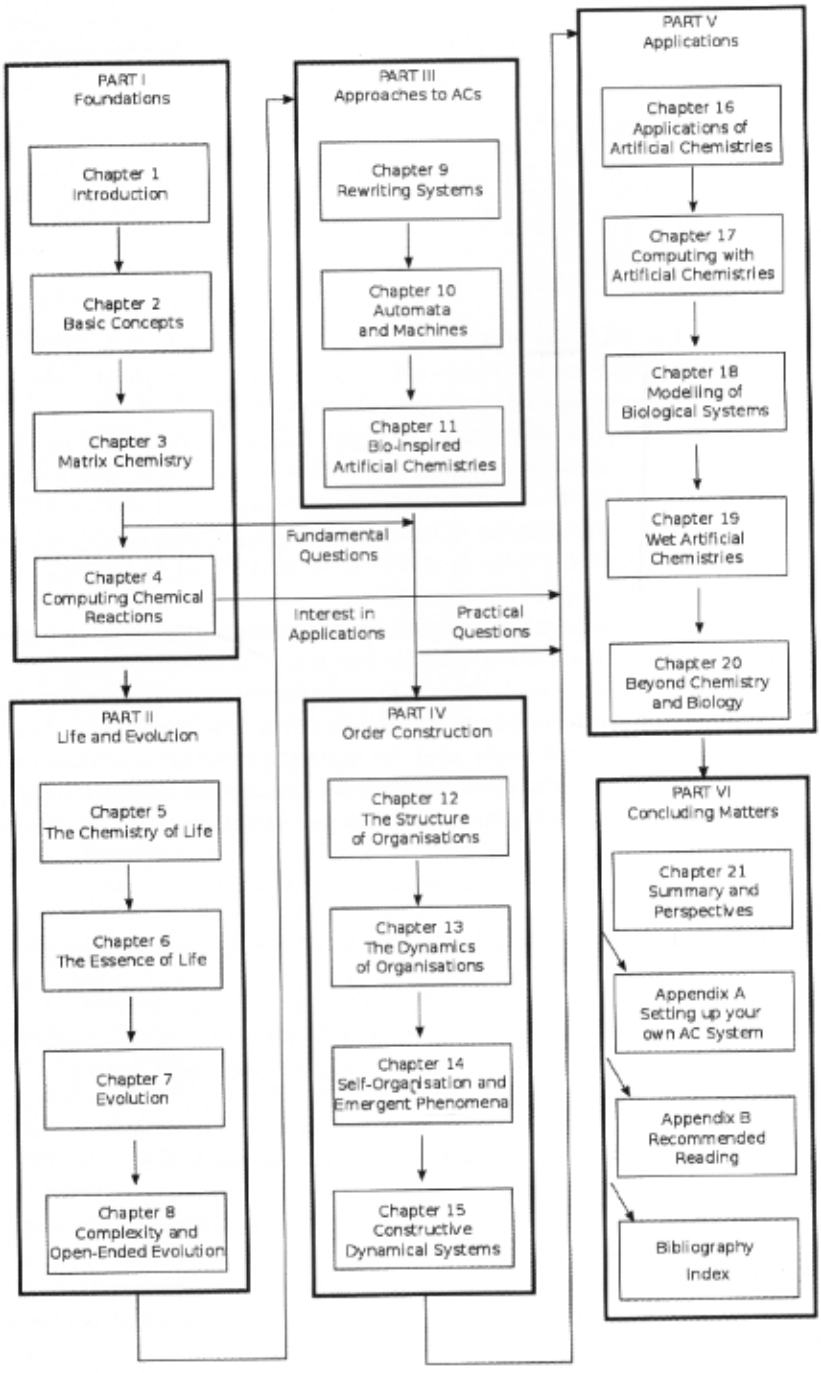
Book Overview

This book will provide an introduction and broad overview of this still relatively young field of artificial chemistries (ACs). The field is highly interdisciplinary, touching chemistry, biology, computer science, mathematics, engineering, and even physics and social sciences to a certain extent. Therefore, we have tried to make the book as accessible as possible to people from these different disciplines. We assume that the reader has some basic knowledge of mathematics and computer algorithms, and we provide a general introduction to the concepts of chemistry and biology that are most often encountered in ACs.

The book will start with a gentle introduction, discuss different examples of artificial chemistries from different areas proposed in the literature, and then delve into a deeper discussion of both theoretical aspects of ACs and their application in different fields of science and technology. An appendix will offer a hands-on example of an AC toolkit ready for the reader to implement his or her own artificial chemistry on a computer.

This book is divided into the following parts:

- Part I holds introductory chapters, with chapter 1 discussing the relation to Artificial Life and other roots of the field, chapter 2 offering a more general methodological introduction,


PART I
Foundations
Chapter 1
Introduction
Chapter 2
Basic Concepts
Chapter 3
Matrix Chemistry
Chapter 4
Computing Chemical
Reactions
PART II
Life and Evolution
Chapter 5
The Chemistry of Life
Chapter 6
The Essence of Life
Chapter 7
Evolution
Chapter 8
Complexity and
Open-Ended Evolution
PART III
Approaches to ACs
Chapter 9
Rewriting Systems
Chapter 10
Automata
and Machines
Chapter 11
Bio-Inspired
Artificial Chemistries
PART IV
Order Construction
Chapter 12
The Structure
of Organisations
Chapter 13
The Dynamics
of Organisations
Chapter 14
Self-Organisation and
Emergent Phenomena
Chapter 15
Constructive
Dynamical Systems
PART V
Applications
Chapter 16
Applications of
Artificial Chemistries
Chapter 17
Computing with
Artificial Chemistries
Chapter 18
Modelling of
Biological Systems
Chapter 19
Wet Artificial
Chemistries
Chapter 20
Beyond Chemistry
and Biology
PART VI
Concluding Matters
Chapter 21
Summary and
Perspectives
Appendix A
Setting up your
own AC System
Appendix B
Recommended
Reading
Bibliography
Index
Fundamental
Questions
Interest in
Applications
Practical
Questions

and chapter 3 exposing, by way of example, key problems that will reappear throughout the book. Chapter 4 gives an introduction to the algorithms applied to chemical reactions, which are also used in ACs.

- Part II, on life and evolution, then steps back for some time to briefly review important aspects of Biology: Chapter 5 discusses the relation between life and chemistry, chapter 6 delves into the essence of life and its origins, chapter 7 reviews the basic mechanisms of evolution and their relation to ACs, and chapter 8 discusses the issue of complexity growth and openness of evolution, a topic that attracts much interest from AC and ALife researchers.

- Part III, Approaches to Artificial Chemistries, is dedicated to a discussion of different Artificial Chemistries introduced in the literature of the last two decades and classifies them into groups: Rewriting Systems (chapter 9) include ACs where the transformation of molecules during "chemical" reactions is dictated by rules that rewrite the contents of these molecules. Automata and Machines (chapter 10) cover ACs that operate in a similar way as a computer with a processor, a memory, and some registers. Bio-inspired ACs (chapter 11) take inspiration from various biological processes, such as the way enzymes operate on DNA molecules.

- Part IV, on order construction, comprises chapters 12 to 15, which expose fundamental questions of how order can emerge. Central to this part of the book is the concept of *chemical organization*, a closed and self-maintaining set of chemicals. Chemical organization theory formalizes this concept and is the topic of chapters 12 and 13. Chapter 12 (co-authored with Pietro Speroni di Fenizio) elaborates on how the structure of organizations can be formalized. Chapter 13 undertakes first steps into the dynamics of organizations. Chapter 14 discusses self-organization and emergent phenomena, which play a key role in ACs. Chapter 15 wraps up with an exposure of constructive dynamical systems, systems that are able to produce novelty and thereby to create new organizations.

- Part V, on applications, returns to reality and is dedicated to a discussion of a broad range of AC applications: Chapter 16 introduces some selected applications; chapter 17 looks at how artificial chemistries can be used for computing; chapter 18 discusses how ACs can be used for the modeling of systems in biology; chapter 19 reports on synthetic life and wet chemical computers; and chapter 20 discusses implementations in different media ranging from mechanical to social systems.

- Part VI concludes the book with a summary chapter (chapter 21), followed by some further suggested reading, and an appendix that introduces a Python toolkit for implementing ACs.

Given the interdisciplinary nature of this book, readers with different backgrounds might find interest in different parts of the book. For instance, readers familiar with chemistry and biology might prefer to skip chapter 5. Readers interested in more fundamental questions will certainly enjoy part IV of the book, while a more practically oriented readership might wish to focus on the application areas in part V. At any time readers should feel free to set up their own AC simulation system. In order to help with that process, we have provided an easy-to-follow guide in the appendix, with code written in Python.

Personal Remarks by Wolfgang Banzhaf

I first became involved with artificial chemistries when I discovered an interest in self-replicating structures. Von Neumann's proof that self-replicating machines are possible, together with the "Game of Life" rules for cellular automata, exerted an enormous influence on me. While those ideas had been established in the 1950s and 1970s, respectively, Artificial Life as a concept took another decade to arrive. At that time I was a freshly minted theoretical physicist, with lots of ideas and no way to realize them.

What is the essence of life? How is it that the molecules in our bodies are replaced every so often, yet we consider ourselves the same, regardless of which molecules are doing their heavy lifting within our bodies? Surely, it could not be the material constitution of our bodies that would make us alive? It was in this context that I began reading books and articles about organization, self-organization, and the processes of life. I realized that below the wonderful phenomena of real life there was a huge machinery of chemical and physical processes, all the time providing the raw material and energy gradients, the driving forces, and the constraints necessary for life to exist.

Following the lead of others, and together with my students, I started to develop notions of artificial chemistry, which at the same time were reinforced and further developed by a whole group of researchers fascinated by Life.

When MIT Press approached me and asked whether I would like to write a book about the topic of artificial chemistries, I was hesitant at first. In a field so new and inhomogeneous as this, how could one hope to find a thread and to provide a concise discussion of the major ideas without sacrificing many of the potentially valuable avenues that are being explored as one writes them down? Fascination with the topic, however, prevailed over caution, and it is in this exploring spirit that we hope you receive this book. It is not intended to discourage any effort in this field — just the opposite, we hope to convey some of this fascination, and to draw as many of you as possible into this field, if you have not yet been dedicated to the cause: to understand life, in all its forms, and therefore ultimately, to understand where we come from.

Personal Remarks by Lidia Yamamoto

When I was invited to help write this book, I felt of course very honored and excited, but at the same time I also felt very scared by the scale of the challenge ahead of me. My enthusiasm finally won over my fear, and I decided to leap at this chance.

Writing this book was a big learning experience for me. Our collaboration was a great pleasure and a source of inspiration for me. This book represents about four years of our joint effort. As I had feared, I was quickly overwhelmed by the huge amount of information that I had to synthesize into a coherent and mature overview of this still burgeoning field. My goal was to make this book as accessible as possible, remembering the person I was when I first came into artificial chemistries, all the questions I had and for which I couldn't find easy answers, and all the questions that I even didn't know how to formulate. One of my past advisors once said that I am a walking question mark. Indeed.

In this book we tried to bring answers to those questions, even if most of the answers consist in saying that no firm answer is currently known, at least we tried to point the reader to the places where people are looking for the answers. We hope that this will stimulate many more people into finding the answers, and then contribute to the progress in the field.

It quickly became apparent that we had to achieve much more than just a big survey of the field of artificial chemistries. This was an opportunity to finally put together the fundamental concepts needed to understand and work with artificial chemistries, the main motivations and rationale behind the work done so far, and where we should be heading from now on. This was a daunting possibility, and perhaps the main value of the book. I don't know if we have attained this ambitious goal; the readers will tell us. However, I think the book at least made a big leap in this direction, although we might not be fully there yet.

Acknowledgments

We are indebted to many people: Bob Prior, executive editor at MIT Press, first planted the idea to consider the plan for a book on artificial chemistries seriously. Susan Buckley, associate acquisition editor at MIT Press, regularly (and patiently) checked in to ask about the status of the book, Christopher Eyer took over from her and helped in the later stages of getting the book draft ready. Katherine Almeida accompanied the production of the book with unfailing diligence.

Over the years, we worked with many individuals (students, colleagues and collaborators) on various aspects of artificial chemistries: Jens Busch, Pierre Collet, Peter Dittrich, Burkard Eller, Mark Hatcher, Christian Lasarczyk, Bas Straatman, Thomas Meyer, Daniele Miorandi, Hilmar Rauhe, Pietro Speroni di Fenizio, Christian Tschudin, Roger White, and Jens Ziegler. We also had many discussions with colleagues in the community who in various ways helped to shape our thinking about Artificial Chemistries or read parts of the book and gave feedback: Mark Bedau, Ernesto Costa, Rene Doursat, Harold Fellermann, Christoph Flamm, Walter Fontana, James Foster, Martin Hanczyc, Stuart Kauffman, Jan Kim, Krzysztof Krawiec, Julian Miller, Una-May O'Reilly, Steen Rasmussen, Hiroki Sayama, Peter Schuster, Lee Spector, Peter Stadler, Brian Staveley, Susan Stepney, Yasuhiro Suzuki, and Hiroshi Tanaka. We gratefully acknowledge the rich and inspiring interactions we had with them all.

Many of our colleagues were so friendly to allow us to reproduce figures from their own work. We have acknowledged these permissions in the appropriate places, but want to express our gratitude here as well to Erwan Bigan, Aaron Clauset, Mark Hatcher, Martin Hanczyc, Simon Hickinbotham, Sandeep Krishna, Thomas Miconi, Robert Pennock, Hiroki Sayama, Peter Stadler, and Sébastien Verel.

This book was typeset in LaTeX's Memoir class and counted upon various tools from the free software and open source communities, including Python, Gnuplot, Inkscape, OpenOffice and many more. We would like to express our sincere gratitude to these developer communities.

W.B. would like to cordially thank his wife Pia for her interest and continuous encouragement in the process of writing this book. L.Y. wishes to thank her husband Pascal for his unconditional support, encouragement, and sacrifices that were essential to her successful contribution to this extensive book writing effort. Both of us are indebted to Pierre Collet from the University of Strasbourg, who kindly provided us with the academic infrastructure needed to pursue part of this project. Finally, we both owe many apologies to our families and friends who were too often neglected on the way toward completion of this project.

Wolfgang Banzhaf, St. John's, Newfoundland, Canada
Lidia Yamamoto, Brussels, Belgium
February 25, 2015