DYNAMICS OF SELF-ORGANIZED AND SELF-ASSEMBLED STRUCTURES

Physical and biological systems driven out of equilibrium may spontaneously evolve to form spatial structures. In some systems molecular constituents may self-assemble to produce complex ordered structures. This book describes how such pattern formation processes occur and how they can be modeled.

Experimental observations are used to introduce the diverse systems and phenomena leading to pattern formation. The physical origins of various spatial structures are discussed, and models for their formation are constructed. In contrast to many treatments, pattern-forming processes in nonequilibrium systems are treated in a coherent fashion. The book shows how near-equilibrium and far-from-equilibrium modeling concepts are often combined to describe physical systems.

This interdisciplinary book can form the basis of graduate courses in pattern formation and self-assembly. It is a useful reference for graduate students and researchers in a number of disciplines, including condensed matter science, nonequilibrium statistical mechanics, nonlinear dynamics, chemical biophysics, materials science, and engineering.

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DYNAMICS OF SELF-ORGANIZED AND SELF-ASSEMBLED STRUCTURES

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University of Toronto
To our families
The dimmed outlines of phenomenal things all merge into one another unless we put on the focusing glass of theory, and screw it up sometimes to one pitch of definition and sometimes to another, so as to see down into different depths through the great millstone of the world.

*Analogies*, James Clerk Maxwell
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Preface

The idea for this book arose from the observation that similar-looking patterns occur in widely different systems under a variety of conditions. In many cases the patterns are familiar and have been studied for many years. This is true for phase-segregating mixtures where domains of two phases form and coarsen in time. A large spectrum of liquid crystal phases is known to arise from the organization of rod-like molecules to form spatial patterns. The self-assembly of molecular groups into complex structures is the basis for many of the developments in nanomaterial technology. If systems are studied in far-from-equilibrium conditions, in addition to spatial structures that are similar to those in equilibrium systems, new structures with distinctive properties are seen. Since systems driven out of equilibrium by flows of matter or energy are commonly encountered in nature, the study of these systems takes on added importance. Many biological systems fall into this far-from-equilibrium category.

In an attempt to understand physical phenomena or design materials with new properties, researchers often combine elements from the descriptions of equilibrium and nonequilibrium systems. Typically, pattern formation in equilibrium systems is studied through evolution equations that involve a free energy functional. In far-from-equilibrium conditions such a description is often not possible. However, amplitude equations for the time evolution of the slow modes of the system play the role that free-energy-based equations take in equilibrium systems. Many systems can be modeled by utilizing both equilibrium and nonequilibrium concepts. Currently, a wide variety of methods is being used to analyze self-organization and self-assembly. In particular, microscopic and mesoscopic approaches are being developed to study complex self-assembly in considerable detail. On mesoscales, fluctuations are important and influence the self-organization one sees on small scales, such as in the living cell. Nevertheless, many common aspects of these pattern-forming processes can be modeled in terms of order parameter fields, which describe the dynamics of relevant collective variables of the system. The patterns
that are formed and the way they evolve are often controlled by certain common elements that include the presence of interfaces, interfacial curvature, and defects.

In order to present an approach to the study of such self-assembled or self-organized structures that highlights common features, we have intentionally limited the scope of the presentation to descriptions based on equations for order parameter fields. Approaches of this type are able to capture the gross features of pattern formation processes in diverse systems, including those in the equilibrium and far-from-equilibrium domains. We have also intentionally omitted descriptions based on various coarse-gained molecular dynamics methods and a variety of other mesoscopic particle-based methods, which are proving to be powerful tools for the study of such systems. In addition, to sharply focus our presentation we have restricted our discussion to systems where hydrodynamic flows are not important.

A selection of the material in this book formed the basis for a one-semester course entitled “Interface Dynamics and Pattern Formation in Nonequilibrium Systems” given jointly in the Departments of Chemistry and Physics at the University of Toronto. Many of the topics covered in the book have been the subjects of intense investigations, and a large literature exists. In order to make the material as self-contained as possible, in most cases we have provided an introduction to each topic in a form that allows the main ideas to be exposed and derived from basic principles. The final chapters of the book provide some additional examples of applications that combine the two underlying themes that are developed in the book: free-energy-functional and amplitude-equation descriptions. These chapters show how the dynamics of physical and biological systems can be modeled using the concepts developed in the body of the book.

Some of the material presented in the book derives from work with our colleagues and students. In particular we would like to acknowledge the contributions of Augustí Careta, Hugues Chaté, Francisco Chávez, Mario Cosenza, Jörn Davidsen, Ken Elder, Simon Fraser, Leon Glass, Martin Grant, Andrew Goryachev, Daniel Gruner, Christopher Hemming, Zhi-Feng Huang, Anna Lawniczak, François Léonard, Roberto Livi, Anatoly Malevanets, Paul Masiar, Alexander Mikhailov, Gian-Luca Oppo, Antonio Politi, Sanjay Puri, Tim Rogers, Katrin Rohlf, Chris Roland, Guillaume Rousseau, Celeste Sagui, Ken Showalter, Kay Tucci, Mikhail Velikanov, Xiao-Guang Wu, Chuck Yeung, and Meng Zhan. We also owe a special debt of gratitude to our colleagues who read and commented on portions of the book: Markus Bär, Jörn Davidsen, Walter Goldburg, Jim Gunton, Christopher Hemming, Zhi-Feng Huang, Chuck Knobler, Maureen Kapral, Alexander Mikhailov, Steve Morris, Evelyn Sander, Len Sander, Celeste Sagui, Peter Voorhees, Tom Wanner, Chuck Yeung, and Royce Zia. The preparation of this book would have been difficult without the help of Suzy Arbuckle and Raul Cunha, and we would like to express our special gratitude to them for their assistance.