

Modeling Chemical Systems using Cellular Automata



Lemont B. Kler
Paul G. Seybold
Chao-Kun Cheng

 Springer



Modeling Chemical Systems Using Cellular Automata

Wayne A. Davis



Modeling Chemical Systems Using Cellular Automata:

Modeling Chemical Systems using Cellular Automata Lemont B. Kier, Paul G. Seybold, Chao-Kun Cheng, 2006-02-23

Modeling Chemical Systems using Cellular Automata provides a practical introduction to an exciting modeling paradigm for complex systems. The book first discusses the nature of scientific inquiry using models and simulations and then describes the nature of cellular automata models. It then gives detailed descriptions with examples and exercises of how cellular automata models can be used in the study of a wide variety of chemical, physical, and biochemical phenomena. Topics covered include models of water, itself, solution phenomena, solution interactions with stationary systems, first and second order kinetic phenomena, enzyme kinetics, vapor liquid equilibrium, and atomic and molecular excited state kinetics. The student experiences these systems through hands-on examples and guided studies. This book is the first of its kind, a textbook and a laboratory manual about cellular automata modeling of common systems in chemistry. The book is designed to be used as a text in undergraduate courses dealing with complex systems and/or as a computational supplement to laboratory courses taught at the undergraduate level. The book includes compact descriptions of a large variety of physical and chemical phenomena. Illustrative examples of simulations with exercises for further study. An instructor's manual for use of the program. The book will be of great value in undergraduate courses in chemistry, physics, biology, applied mathematics, and bioinformatics and as a supplement for laboratory courses in introductory chemistry, organic chemistry, physical chemistry, medicinal chemistry, chemical engineering, and other courses dealing with statistical and dynamic systems. It allows the exploration of a wide range of dynamic phenomena, many of which are not normally accessible within conventional laboratory settings due to limitations of time, cost, and experimental equipment. The book is both a textbook on applied Cellular Automata and a lab manual for chemistry, physics, engineering courses with lab activity. It would supplement other lab work and be an additional book the students would use in the course. The authors have assessed the emerging need for this kind of activity in science labs because of the cost of the practical activities and the frequent failure of some exercises leading to lost didactic value of some experiments. This book is pioneering an alternative that will grow in use. There are no course directors who would use Cellular Automata exclusively. The authors see an emerging interest in this kind of work in courses that contain lab exercises. One such course is the graduate course that Lemont Kier gives in Life Sciences about complexity. He uses many examples and studies from Cellular Automata in the latter part of this course.

Cellular Automata Dooyne Farmer, Tommaso Toffoli, Stephen Wolfram, 1984 Australian Journal of Chemistry, 2006 Advanced Manufacturing Systems, ICMSE 2011 Dao Guo Yang, Tian Long Gu, Huai Ying Zhou, Jian Min Zeng, Zheng Yi Jiang, 2011-02-21. Selected peer reviewed papers from the International Conference on Manufacturing Science and Engineering ICMSE 2011 9-11 April 2011 Guilin, China Chemical Evolution--self-organization of the Macromolecules of Life Julián Chela Flores, 1995. The contents record evidence of early life from the oldest known fossil in the geological record as well as the prior events of chemical

evolution the question of the chirality of protein amino acids is discussed The book is organized in five sections corresponding to chemical geological biochemical biophysical aspects of self organization concluding with a section on chirality It provides an excellent introduction to this ever growing interdisciplinary area of research in chemistry physics the life sciences This volume is a Festschrift for the late Professor Cyril Ponnamperna in whose honor the Second Trieste Conference was held contains the papers presented at the Conference

Cellular Automata Modeling of Physical Systems Bastien Chopard, Michel Droz, 2005-06-30 This book provides a self contained introduction to cellular automata and lattice Boltzmann techniques Beginning with a chapter introducing the basic concepts of this developing field a second chapter describes methods used in cellular automata modeling Following chapters discuss the statistical mechanics of lattice gases diffusion phenomena reaction diffusion processes and non equilibrium phase transitions A final chapter looks at other models and applications such as wave propagation and multiparticle fluids With a pedagogic approach the volume focuses on the use of cellular automata in the framework of equilibrium and non equilibrium statistical physics It also emphasises application oriented problems such as fluid dynamics and pattern formation The book contains many examples and problems A glossary and a detailed bibliography are also included This will be a valuable book for graduate students and researchers working in statistical physics solid state physics chemical physics and computer science

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