Preface

Today a small army of physicists, chemists, mathematicians, and engineers has joined forces for a renewed attack on a classic problem, the "reversibility paradox". The paradox is simply stated: "How can the *irreversible* Second Law of Thermodynamics be compatible with, and result from, an underlying *time-reversible* mechanics?" Building on the ideas of van der Waals and Maxwell, Boltzmann provided the classic nineteenth-century resolution of the paradox by using a probabilistic analysis of dilute-gas collisions. Here I bring Boltzmann's classic analysis up to date by adopting modern tools. This approach augments and generalizes Boltzmann's statistical understanding. The new interpretive tools are (i) Linear-response theory, a consequence of Gibbs' statistical mechanics, (ii) Chaos theory and (iii) the Fractal geometry to which it leads, and (iv) Computers, which make possible the simulations and analyses which were not available to Boltzmann. As the available tools change, so do the targets and the points of view. Philosophers interested in the reversibility paradox have provided some insight too. We will seek correlations with their work.

The present book describes both the scientific and the philosophical work from the perspective of computer simulation, emphasizing my own *thermo*mechanical approach to resolving the reversibility paradox by analyzing the consequences of time-reversible thermostats. Computer simulation has made it possible to probe and characterize time reversibility from a variety of directions. "Chaos theory" or "nonlinear dynamics" has supplied a vocabulary detailing a useful set of concepts, which allows for a fuller explanation of irreversibility than was available to Boltzmann or even that provided by the linear response theory of Green, Kubo, and Onsager.

Throughout my own research career I have spent countless hours rereading the fruits of others' work. This rereading has been made necessary by the lack of clear example problems illustrating the meanings of the concepts used in these works. While this lack was understandable in the precomputer era of Boltzmann, Krylov, and Zubarev, it is inexcusable today. Throughout the book I emphasize the clear illustration of fundamental concepts with simple example problems, suited to desktop computation. I have also clarified the concepts by including a glossary of technical terms from the specialized fields which are combined here to focus on a common theme.

I am personally quite satisfied with the modern resolution of the reversibility paradox, as presented here. I see thermodynamic irreversibility as an inevitable, understandable outcome of an underlying time-reversible dynamics. This understanding is predicated on accepting that *no* dynamics is a *perfect* replica of nature. I cannot imagine any completely comprehensive "unified theory", able to include all of nature, together with its observers. My goal, in this book, is more modest. I wholeheartedly embrace *classical* mechanics as the most useful basis for an understanding of the physical world on the length and time scales relevant to us humans. By generalizing classical mechanics, to include temperature and thermostated "thermal boundaries", we obtain "thermomechanics". This discipline will be our main model for the exploration and explanation of the links between time-reversible micromechanics, macroscopic irreversible thermodynamics, computer simulation, modern chaos theory, and fractal geometry.

The book begins with a discussion contrasting the idealized deterministic reversibility of basic physics with the pragmatic unpredictable irreversibility of what we call "real life" or "nature". The chaotic complexity discovered by Maxwell, Boltzmann, and Poincaré suggests that the unpredictability of life is intrinsic. This view is quite consistent with Gödel's undecidability proof, as well as with our quite evident ability to affect the future by exercising "free will".

Computational models and simple thermomechanical simulations based on them are discussed and illustrated throughout the book. The simulations provide a reliable means to assimilate complex concepts through worked-out examples. Such analyses, from the point of view of dynamical systems, are applied to simple two-dimensional maps and higher-dimensional dynamical systems, as well as to many-body examples from nonequilibrium molecular dynamics and to chaotic irreversible flows from finite-difference, finite-element, and particle-based continuum simulations. Two necessary concepts from dynamical systems theory—fractal distributions and Lyapunov instability—are fundamental to interpreting the results of the computational approach.

Undergraduate-level physics, calculus, ordinary differential equations, and a taste for computation are sufficient background for a full appreciation of the book. For nearly twenty years the Academy of Applied Science (Concord, New Hampshire) has sponsored the summer work of bright high-school seniors in the University of California's Davis Campus' Department of Applied Science at Livermore. The example problems worked out in the book are representative of the summer projects to which these students have contributed. The book is intended to appeal to advanced undergraduate as well as to graduate students, and to research workers. I fervently hope that the generous assortment of examples that I have worked out in the text will stimulate readers to explore and enjoy the rich and fruitful field of study which links fundamental reversible laws of physics to the irreversibility which surrounds us all. I have chosen mainly one- and two-dimensional examples in order to permit me to convey ideas with simple *pictures.* I stress here that the *ideas* so illustrated are not essentially different in three space dimensions.

To summarize the view I have reached, as the result of a decade of research, the Second Law of Thermodynamics is most simply described as a ubiquitous time-symmetry breaking which invariably accompanies the dynamics of a sufficiently chaotic system connected to its environment. Now it is certainly true that the "chaos" and symmetry breaking found in computer simulations are idealizations of the chaos and irreversibility of "nature". Our simulations are classical and nonrelativistic. They have a finite and digital representation. Nevertheless it *is* well-established by now that computational "pseudochaos" provides results which show no important differences from the idealizations of nature in the minds of mathematicians and the real-world observations of experimentalists.

Some of the popular books dealing with chaos and irreversibility seek an understanding of the macroscopic irreversibility of nature in terms of a comprehensive quantum mechanical and cosmological explanation, by linking the present state of the Universe to its "initial conditions". To me it is completely implausible that particular initial conditions, cosmological or not, are at all relevant to understanding the irreversibility present in everyday diffusive, viscous, or conducting flows. None of these ambitious books takes seriously the need for including boundary conditions and constraints in dynamics, which seems to me a crucial ingredient to obtaining irreversible behavior from time-reversible laws. It is clear that computer simulation has been the catalyst for our new understanding of irreversible flows.

There are *many* books addressing irreversibility. Most of them at least mention computer simulation. But there are really only two, Evans and Morriss' *Statistical Mechanics of Nonequilibrium Liquids* and my own *Computational Statistical Mechanics*, which emphasize the primary importance of simulation to a proper understanding of the "reversibility paradox" and the involvement of fractal distributions in resolving it. More mathematical expositions of some of the underlying ideas can be found in Dorfman and Gaspard's books. More philosophical expositions include Coveney and Highfield's, Dudeney's, Hawking's, Penrose's, Price's, and Sklar's. For me, Sklar's is the most interesting of all of them. He emphasizes the classical aspects of the reversibility paradox while simultaneously exploring and expounding a wide variety of alternative points of view.

My own approach is, I think, much the simplest, and proceeds by way of defining nonequilibrium states, in order to reach a compelling understanding of *irreversibility* in terms of the straightforward, but subtle, consequences of *time-reversible* chaotic differential equations. Generating the nonequilibrium states *via* computer simulation is illustrated here in the many example problems. It is my fond hope that the reader will find this approach palatable.

I would like to thank Richard Lim and Robert MacKay for stimulating and encouraging the effort needed to write this book. I also owe a longstanding continuing debt of thanks to my colleagues, friends, and students, for helping me to understand, and to the Livermore Laboratory, the University of California, and universities in Australia, Austria, Germany, Japan, Korea, and Poland, for having provided me with the resources and havens necessary to teaching, research, and good fellowship.

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Hideout Canyon Ranch–Red Skunk Ranch, 1998–1999
Stanislaus and Santa Clara Counties, California, USA