are included. The microscopic analogs of these sources and sinks require generalizing the purely-Newtonian mechanics familiar to physicists.

The familiar irreversible processes which are all around us are not at all similar to the near-equilibrium fluctuations exploited by linear-response theory. Linear-response theory deals with ensemble-averaged infinitesimals. Macroscopic irreversible processes are individual and strongly driven, far from equilibrium, and inherently complex. These far-from-equilibrium conditions require special computer simulation techniques.

1.7 Reversibility Paradox: Irreversibility from Reversible Dynamics

The conflict between basic time-reversible physics and applied irreversible engineering is the "reversibility paradox". For gases, Boltzmann clarified this paradox by showing that averaging, justified by collisional chaos, was an essential part of its resolution. He showed that a statistical averaging of collisions, which ignores any pre-existing correlations and fluctuations, converts the reversible equations governing low-density gas dynamics to the irreversible equations of continuum mechanics. His approximate Boltzmann equation¶, for the evolution of the single-particle probability density, f_1, makes detailed predictions for the approach to equilibrium, and for the velocity distributions characterizing systems undergoing diffusive, viscous, and conductive dissipation. For dilute gases, the time-development of Boltzmann's approximate single-particle entropy,

$$S_{\rm B}(t) \equiv -Nk\langle \ln f_1 \rangle \equiv -k\textstyle\int dr \int dv f_1(r,v,t) \ln f_1(r,v,t),$$

agreed with the predictions of irreversible thermodynamics, opening the way for Gibbs' formulation of statistical mechanics for general systems, but restricted to equilibrium.

Green and Kubo showed that Gibbs' averaging links the irreversible transport coefficients of phenomenological continuum theory to the decay of equilibrium fluctuations. For dilute gases, these results are also equivalent to Boltzmann's. After Green and Kubo discovered linear-response theory, theoretical progress was stalled, awaiting the development of fast computers. The need to understand complex chaotic behavior frustrated

¶ $\dot f_1 \equiv (\partial f_1/\partial t)_{\rm collisions}$. The approximate collision term, $(\partial f_1/\partial t)_{\rm c}$, is *quadratic* in f_1.

the attempts of analysts. Computers made progress possible again. Recent numerical work has shown that even *few*-body systems show irreversible behavior, on the average, even with rigorously time-reversible motion equations. The irreversibility emerges with great clarity and precision when the small-system results are time averaged.

Computers made it possible to simulate both reversible mechanics and irreversible flows. In the latter case it was necessary to impose boundary conditions or constraints, driving the system from equilibrium. Heat and work had to be incorporated explicitly into the programming. Handily, all this could be done without sacrificing the time reversibility of the underlying equations!

1.8 Example Problems

To illustrate the concepts of time reversibility and chaos we consider here three examples. The first is a two-dimensional area-preserving map. It is a caricature of equilibrium flows obeying Liouville's incompressible theorem. The second is a three-dimensional continuous flow, but with *discontinuous* forces and a simple phase-space structure. The last is a three-dimensional flow with continuous forces and a *complicated* phase-space structure. All three of these problems can exhibit chaotic behavior, with small changes in initial conditions growing exponentially with time. All three are relatively easy to simulate and to visualize. Each is a building block in creating an understanding of the nonequilibrium systems which are emphasized in the following Chapters of the book. The underlying background in mechanics and numerical algorithms, required to generate numerical solutions for the last two problems, is given in Chapter 2.

1.8.1 *Equilibrium Baker Map*

If N coordinates suffice to represent a system's configuration then the configuration at any fixed time is represented by a single point in the corresponding N-dimensional space. The time development of that point defines a one-dimensional "trajectory"—a line—in that same space. Imagine the repeated intersections of such a trajectory with some fixed $(N-1)$-dimensional surface embedded in the N-dimensional configuration space. The successive intersections with such a surface provide a "Poincaré Sec-