The misguided emphasis on initial conditions likewise ignores the empirical basis of physics. Experiments are useful aids to understanding precisely because microscopic initial conditions are quite irrelevant to the macroscopic outcome. If initial conditions *were* crucial there could be no bodies of knowledge, like physics and chemistry, which describe the evolution of macroscopic behavior independently of the microscopic details.

In addition to this justifiable complaint, choosing the "right" initial conditions appears hopeless whenever, as is usual, the dynamics is "sensitive to initial conditions", meaning Lyapunov unstable. By "Lyapunov instability" I refer to the pervasive growth, exponential in time, of small perturbations of the initial conditions. More details are given in Sections 1.5 and 7.4. In principle Lyapunov instability implies that choosing the "right" initial conditions requires an *infinite* amount of information. This requirement, a consequence of precisely defined trajectories, is *meaningless* from any operational point of view. In practice, double-precision simulations are limited to an uncertainty of about 10^{-28} per coordinate-momentum pair, similar to the uncertainty which governs real experiments when the masses, lengths, and times are respectively of order grams, centimeters, and seconds. This latter observation follows from Heisenberg's "uncertainty principle", and guarantees that any precise effect on the atomic level, due to initial conditions, would disappear in just a few interatomic collision times. A perceptive discussion appears in Ruelle's delightful book *Chance and Chaos*. Double precision is coincidentally also the right choice for continuum simulations, in which microscopic fluctuations of order 10^{-14} are to be ignored.

1.2 Time-Reversible Theories of Irreversible Processes

"Sensitivity to initial conditions" suggests, first of all, that no theory can be judged reasonable if its physical predictions depend sensitively upon the initial data. "Sensitivity" also suggests that a changed less-sensitive theory, perhaps with a more limited goal, might well do better. Such theories can be developed by focussing on another aspect of the solution process, the interaction of the system with its surroundings, as modelled in computer simulations by boundary conditions, constraints, or driving forces. Nonequilibrium systems are typically *open* or *driven* systems, with external sources and sinks of mass, momentum, and energy. Though such systems are more complex than the idealized isolated systems of Newtonian mechanics, the cost of describing this additional complexity is justified by the wide scope of new problem areas such a generalized approach can explore. The simplest useful microscopic models for understanding the everyday world of human experience are time-reversible dynamical theories which include nonequilibrium boundary conditions, constraints, and driving forces.

From both standpoints, computational and analytical, the best physical theories from which to start are (i) the simplest microscopic theory of particle motions, classical mechanics, and (ii) the macroscopic theory of continuum mechanics. Classical mechanics, with boundary conditions, constraints, and driving forces, presently provides a comprehensive description of a wide range of motions, generally thought of as including both the reversible *and* the irreversible types, and ranging in scale from the microscopic level of atomistic mechanics to the macroscopic levels of structural engineering and astronomy. Classical mechanics is a fairly faithful description of physical reality, simpler, and closer to human experience, in most cases, than is its quantum cousin.

A growing appreciation of the complexity inherent in simple theoretical structures has revealed that the task of constructing a comprehensive "unified theory" of "everything" is unattainable. For this reason it is logical to follow Occam's lead, using the philosophical principle of "Occam's Razor" to cut away all but the simplest parts of the candidate theories describing the phenomena of interest. Mechanics, when coupled with boundary conditions, constraints, and driving forces, is enough to explain the symmetry-breaking associated with irreversible processes, and to resolve the conceptual problems associated with conservative mechanics. I like to call the augmented mechanics "thermomechanics" to emphasize its link to thermodynamics and nonequilibrium flows through the explict incorporation of thermal effects.

Thermomechanics is a direct outgrowth of computation and simulation. When fast computers became generally available, in the 1960s, new problem areas opened up and old analytic approaches could be gracefully abandoned. By the early 1970s, thermomechanics had come into its own as a direct result of computation. Nonequilibrium molecular dynamics was developed in 1972. Nosé's discovery of time-reversible thermostats matching Gibbs' canonical ensemble came in 1984. Much of the subsequent work was devoted to checking that the new methods agreed with Gibbs' statistical equilibrium predictions, as augmented by Green and Kubo's exact formulation of linear transport processes. Direct computer simulation replaced virial series for the pressure and integral equations for the distribution of particle pairs as the simplest path to equilibrium properties. Likewise, computer algorithms largely replaced the construction and analysis of "kinetic equations" for *non*equilibrium problems. The resulting extensions of mechanics to the definition and exploration of *nonequilibrium* systems with special boundary conditions, constraints, and driving forces, would have been incomplete and unrewarding without the computers necessary to solve the underlying differential equations. Let us begin to explore computer simulation by describing the application of fast computers to the task of solving the mechanical motion equations for both microscopic and macroscopic systems.

1.3 Classical Microscopic and Macroscopic Simulation

In classical continuum mechanics, the usual space-and-time-dependent variables are the mass density, velocity, and energy per unit mass,

$$\{\rho(r,t), v(r,t), e(r,t)\}.$$

The motion of a continuum is in principle more complex than that of a system of particles because the dependent variables $\{\rho, v, e\}$ must be known *everywhere*. The time evolution of this set reflects the interdependent flows of mass, momentum, and energy in response to the fields and gradients driving them.

Typical macroscopic computer simulations contain irreversible "constitutive relations". There are two different reasons for this. First, much of the irreversibility we see around us *can* be explicitly and accurately simulated by including Newtonian viscosity and Fourier's heat conductivity. Second, an enhanced *artificial* irreversibility must often be used (artificial viscosities and conductivities are examples) to stabilize numerical techniques. In either case, with "realistic" or "artificial" irreversibility, the simulations are complicated whenever nonlinear effects, leading to chaos, are included. The solutions of the irreversible macroscopic equations can closely resemble the results of laboratory experiments. But, due to their intrinsic irreversibility these macroscopic simulations are often viewed as "less fundamental" than time-reversible microscopic simulations based on particle mechanics. The main criticism levelled at the macroscopic approach *is* its lack of time reversibility. A subsidiary and related aspect of the macroscopic approach