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 is its exclusion of certain fluctuations. The averaging which results in this exclusion has two effects: besides destroying time reversibility it eliminates the complexity associated with extraneous microscopic degrees of freedom. It is only in problems where this complexity is important, like turbulence, that pursuit of the macroscopic approach is bogged down by the complexity characteristic of microscopic representations. The probabilistic nature of quantum mechanics suggests a kind of "averaging" too, but, unlike macroscopic mechanics, Schrödinger's quantum mechanics is completely time-reversible.

Computer simulation solves problems in a way which was novel at the time of the Second World War, and which still meets occasional pockets of resistance. The analytical textbook style of problem solving gives a "solution" described by orthogonal polynomials or series expansions. The computational approach *simulates* the *evolution* of a physical system. The polynomials and expansions are replaced by computer *algorithms.* The computational solution is most likely a time-ordered sequence of coordinate data, supplemented with the evolving values of field variables (stress, heat flux, temperature, and the like). In classical particle mechanics, the trajectories $\{r(t)\}$ describing a solution of Newton's equations $\{F = m\ddot{r}\}$ provide also a reversed, second solution, of the *same* equations, obtained by tracing out exactly the same coordinate values. but in a time-reversed order. In such a time-reversed solution, $\{r(-t)\}$, the particle velocities $\{v \equiv \dot{r} \equiv dr/dt\}$ all change sign, but still obey Newton's equations linking the forces, masses, and accelerations.

How could such a symmetric time-reversible situation reliably describe the irreversible phenomena of the real world? There are several approaches to answering this paradoxical question. But, since the only missing ingredient is the set of initial conditions from which the solution is to be continued, it has been common to "explain" the irreversible behavior by pointing to the special nature of the initial conditions. There is a flaw to this misguided explanation. That flaw is chaos, introduced in the next two Sections and discussed at greater length in Chapter 7.

1.4 Continuity, Information, and Bit Reversibility

Newton's ordinary differential equations of motion describe the motion of mass points subject to forces. The motions which result, $\{r(t)\}$, are typ-