

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-

ically continuous flows with smooth time derivatives, $\{v(t) = \dot{r}\}$, which obey Newton's differential equations of motion: $\{a = (F/m) = \dot{v}(t) = \ddot{r}\}$. Because the equations are typically nonlinear, and beyond the reach of analytic techniques, a closed-form solution of these equations, giving the particle coordinates as explicit functions of the time, is generally not possible.

As discussed in Section 1.2, the presence of *chaos* in the solution suggests an explanation for the lack of analytic solutions. As time goes by, the "information"—the number of binary bits—required for an accurate analytic solution grows linearly with time. Eventually the required information lies beyond the capabilities of analysis and computation. The gross features of the present and future come to depend upon finer and finer features of the far distant unknowable past. No conceivable improvement of the spatial and temporal resolutions can overcome this problem. The fundamental reason is sobering. It is characteristic of chaotic systems that the most precise experiments or most-carefully-designed simulations cannot probe the future reliably for more than a few collision times. Thus the "determinism" of mechanics is an illusion[†]. It is the *irrelevance* of the initial conditions (due to the randomizing effects of chaos) which makes the systematic study of physics possible. This randomizing—also referred to as "mixing"—corresponds to information loss. As time goes by the link between present and past becomes more tenuous.

A numerical solution of Newton's equations is typically approximate, with limited fourteen-digit precision. The contrast between an ideal continuous solution $\{r(t)\}$, with both the coordinates and the time continuous and precisely known, and a doubly-discretized computer-generated numerical approximation is sharpest if one imagines a solution space in which points are restricted to a regular spatial grid and are evenly spaced in time $\{r(n\Delta t)\}$. In Chapter 2 we discuss Levesque and Verlet's construction of "bit-reversible" doubly-discretized solutions which are *rigorously time-reversible*. Any such numerical trajectory is necessarily periodic, while a continuous trajectory would have to satisfy very special initial conditions in order to achieve periodicity. The *inevitable* periodicity associated with a discrete solution space suggests that such a space cannot be used to describe irreversible flows in isolated systems. Order of magnitude estimates suggest that Poincaré recurrence times are of order $\sqrt{e^{S/k}} = \sqrt{\Omega}$ in a discretized

[†]As was well known to Maxwell and Poincaré.

space with Ω discrete states. Such times are effectively infinite (exceeding the Age of the Universe) once the number of particles is of order ten to a hundred. Despite the formal periodicity it is quite possible to describe Lyapunov instability, the sensitivity to small perturbations called “chaos”, using the bit-reversible approach.

1.5 Instability and Chaos

Turbulence has long been singled out as a specially “difficult” subject. This characterization of turbulence has arisen from the continuing failure of attempts to predict, or at least to understand, the long-time behavior of complex flows, such as our weather, despite the well-recognized importance of the task. Turbulent instability occurs whenever the decay rate associated with fluid deformations—changes in shape—is sufficiently small. In 1963 Lorenz described his efforts to continue the numerical solution of his now-famous set of three differential equations[§], starting out from intermediate values. He found that this second solution failed to agree with his original one after a fairly short time. Further investigation showed that the mechanism for the disagreement was the *exponentially* unstable loss of information, with the precision required to reproduce a solution of fixed accuracy increasing *exponentially* with the required time, corresponding to the required number of decimal *digits* or binary *bits* increasing *linearly* with time. With Lorenz’ work it became “widely known” (to experts) that *most* flows contain this same sensitivity, “Lyapunov instability”, to small changes in initial conditions.

Quite typically, both microscopic and macroscopic equations of motion are Lyapunov unstable, meaning that their solutions are very sensitive to small perturbations, so sensitive that such perturbations grow *exponentially* fast, in time. Though it is completely deterministic, and in principle reproducible, the chaos which characterizes Lyapunov instability means that particular precise initial conditions are not a useful concept. This is just as well, inasmuch as the concept of a completely isolated system has no sound basis in physics, where everyday gravitational forces have infinite range. On the other hand, *gross* characteristics of initial conditions *do* describe the spatial variations of macroscopic features, such as the temperature or

[§] $\dot{x} = -\sigma(x - y)$; $\dot{y} = \mathcal{R}x - y - xz$; $\dot{z} = xy - bz$. See Section 4.9.1 for more details.