I. Emerging Complexity, Order and Chaos

This introductory section to the Statistical Theory course is meant to illustrate scientific insights that appear to contradict our daily experience of macroscopic objects and dynamical processes. We understand the simple trajectories of tennis balls or of planetary motion due to a simple force, gravitation, the general attraction of massive bodies towards each other. On the other hand, one suspects that the rules that govern the growth and replication of organisms, of polymerization of organic molecules, or of the birth and demise of entire galaxies, are very complex. Simple rules should lead only to simple structure and simple, predictable behavior. Intricate structure and processes, so it seems, are caused by complex underlying rules, possibly by the cooperation or competition of many different laws. It is not immediately obvious, if and how these two regimes of (minimal and maximal) complexity are related to each other, but related they are.

Progress made by science in recent years, studying behavior and evolutionary adaptation to environment by simple and complex systems, has demonstrated that there is really no fundamental difference between systems that behave orderly, in a predictable fashion, and chaotic systems, which evolve in an entirely unpredictable fashion. Neither is it true that simple laws cannot lead to complex behavior or intricate structure. In fact, as it turns out, the only plausible way to produce complexity in nature is through progressive evolution in time of initially very simple systems governed by very simple natural laws.

The following sections illustrate a few examples of transitions from order to chaos and back in dynamic systems that can be modeled by simple mathematics. It is also shown how complexity can emerge from simple underlying rules or laws of replication which through selectivity can become adaptive.

1. General Considerations

The roots of modern science go back to the 17th and 18th centuries, initiating a period of **Enlightenment**, where previous dogmas were reviewed in the light of experimental knowledge and critical rationality. This period had a profound impact on the view of Nature held by the inhabitants of Western Culture and their organization of society. The success of the new mechanistic science suggested that the whole universe was in **well-ordered**, causal motion governed by **quantitative** and relatively simple, knowable physical laws.

Figure 1: Isaac Newton

Newton was one of the important architects of the new science. Newtonian physics says that future mechanical motion is **accurately predictable** from the presence, if the acting forces and inertias associated with a system are precisely known. Any uncertainties are then entirely due to a lack of knowledge, for example, about the system's **initial conditions**. Taking a relatively narrow view of the physical regularities of mechanical motion, discovered in the 17th century, led to the picture of the universe as a giant clockwork of wheels and gears. Well-known illustrations are mechanical models of the planetary system used for demonstration purposes.

Figure 2: Henrie Poincaré

Such a simple mechanical model of the universe never works perfectly. It requires frequent resetting and synchronization with the actual motion of the planets. The inadequacy of Newtonian mechanics for a description of the planetary system was noted first in the 19th century by **Henrie Poincaré**. He described the impossibility to solve accurately the simple **3-body problem**, e.g., the motion of a small satellite around a heavy planet and a massive star (see simulation). He found an unexpected, very high **sensitivity** of the satellite's trajectory **to initial conditions,** represented by the positions and velocities of the interacting masses. Small changes in these conditions led to dramatically different trajectories. The trajectories themselves were not at all **orderly**. They did not correspond to periodic motion on a stable orbit. Many trajectories were highly irregular or **"chaotic"**. To find stable, orderly orbits in a system of 3 or more bodies has remained a challenge to modern science still to date. Chaotic motion has now also been definitively identified in our planetary system, examples are the trajectories of various **moons of Jupiter**.

Coupled Pendulum

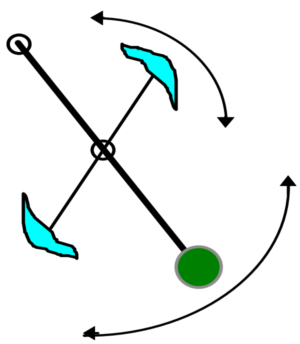

Figure 3: Coupled pendulum capable of

Lorenz' Convective Roll

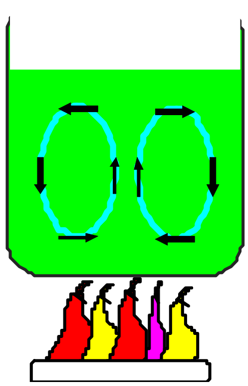

Figure 4: Convective currents in a beaker on a hotplate.

While it is not so easy to demonstrate actual planetary motion, chaotic behavior can be observed with many relatively simple mechanical systems. One example is a magnetic pendulum swinging erratically in the field of several other magnets. Another example is a **coupled pendulum** kicked periodically by a magnet in the base of its stand. One expects that, after a few initial forced oscillations, the motion of the coupled pendulum would settle to be a completely predictable motion about some equilibrium point in space. This is actually not the case, since the smaller pendulum sometimes moves in a synchronized fashion with the driving pendulum but can suddenly undergo an erratic back-and-forth motion.

Such behavior is now understood to result already for 1D motion, if it is governed by a non-linear force, a force that does not increase in proportion to displacement from the equilibrium point. Chaotic behavior can also be expected for motion along several degrees of freedom, when there is a strong **feed-back mechanism** coupling the different degrees of freedom. This latter situation applies to the above coupled pendulum (Fig.3). It also applies to the case of a beaker filled with liquid on a hot plate, in which the temperature difference from bottom to top drives a **"convective roll"**, which tends to change just this gradient. This situation has been studied by **Edward Lorenz** in 1963, who tried to understand the atmospheric flows determining the weather and discovered the phenomenon of chaos instead. He set up the following coupled differential equations for the velocity (*x*) of rotation of the flow, the temperature difference (*y*) between ascending and descending currents, and the deviation (*z*) of the vertical temperature profile from a linear law:

Figure 5: Edward Lorenz, discoverer of chaotic weather patterns.

$$\frac{dx}{dt} = a \cdot (y - x) \qquad \frac{dy}{dt} = r \cdot x - y - x \cdot z \qquad \frac{dz}{dt} = -b \cdot z + x \cdot y \tag{1}$$

where *a, b,* and *r,* are non-negative constants and *t* is the time. The coordinate triplet {x(t), y(t),z(t)} then indicates a time dependent system trajectory.

From Equs. (1), one observes that the convective flow *x* is driven by the temperature gradients (*y* and *z*). For example, for a constant temperature difference *y*, e.g., $y \equiv 0$,

$$x(t) = x(t = 0) \cdot e^{-at} \tag{2}$$

the rotation would slow down exponentially in time. On the other hand, these gradients are created and changed by the convective flow (roll). As a result, the liquid in the beaker can exhibit an orderly flow pattern or chaotic behavior, depending on the values of the parameters. These values can be changed by changing the heat influx into the liquid or the properties of the substance.

Interpreting the Lorenz variables *x, y,* and *z* as the Cartesian coordinates of points in a three-dimensional space and Equs. (1) as equations of motion for the three components {*x(t), y(t), z(t)*} of successive points on the time-dependent system "trajectory" or "orbit", one can reconstruct such orbits for different values of the parameter set [*a, b, r*] by “integrating” the differential equations of motion:

$$x(t+\Delta t) = x(t) + \left(\frac{dx}{dt}\right)\Delta t \qquad (3)$$

and similarly for *y* and *z*.

A program (***CHAOS***) is available that integrates the equations of motion for Lorenz' weather model. For many parameter sets, i.e., for low heat supply and low temperatures, the Lorenz weather orbit settles down to a single point in space {*x, y, z*}. These points are called "**attractors**". Here, the system is stable, exhibits a convective roll with a constant roll velocity *x* and constant temperature differences *y* and *z*.

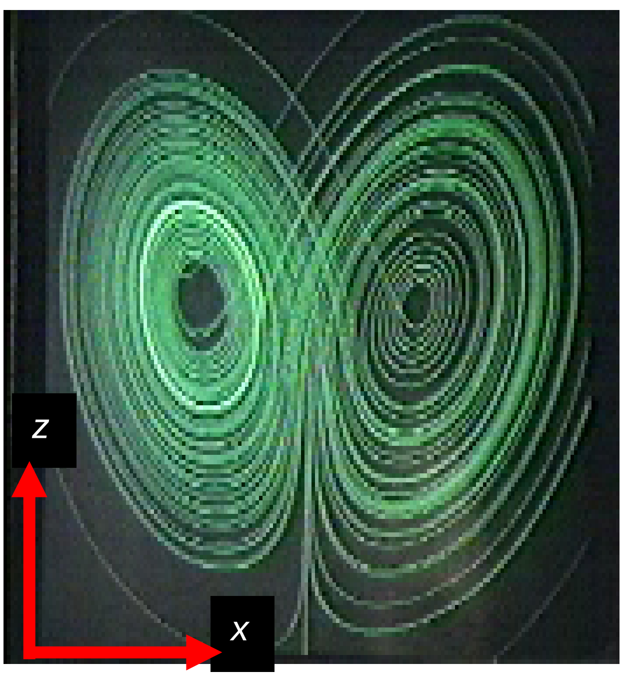

Figure 6: Trajectories in Lorenz' weather model populate two domains in {x,y,z}.

For others parameter sets the orbit oscillates back and forth between two different domains in the space {*x, y, z*}, for example, the sense of the roll changes direction every so often (animation). Interesting orbits result for the parameter set [*a= 10, b = 8/3, r = 28*]. The figures show such orbits viewed from a point on the *x*-axis (top), one on the *y*-axis (middle), and one on the *z*-axis. The figures were generated with the *CHAOS* program. The two different domains are well distinguished.

They are called "**basins of attraction**".

Sensitivity to initial conditions is illustrated in another animation.

Another situation leading to chaotic dynamics is present when forces acting on the system are **non-linear**. This is the case, for example, when the restoring force (tension) of a spring does not increase in proportion to its elongation, or when a force accelerating a mechanical body depends on the velocity of this body. Generally, **complexity** of a system implies either or both conditions, making the system behave orderly or chaotically. Examples of such systems are macroscopic containers filled with gases of many atoms or molecules, or even microscopic clusters containing a number (≥ 3 *!!*) of constituents and atomic nuclei.

It is the type of chaos due to complexity that is responsible for the macroscopic behavior of gases and liquids, as well as for many aspects of reactions between molecules, atoms, or nuclei. Although it is, in principle, impossible to make predictions for the precise state of systems such as gases, the **average behavior** of these systems is predictable, as well as the magnitude of (average) **fluctuations** about this average. The average behavior of substances is the object of **Thermodynamics**. It is the task of **Statistical Mechanics**, to give an explanation of for this macroscopic behavior in terms of the underlying microscopic structure of the system.

It is not self-evident, how a deterministic microscopic motion can lead to unpredictable macroscopic behavior in which a single, erratic system trajectory can cover a sizable fraction of the total accessible phase space. Therefore, a simple experiment will be discussed first, which can exhibit both orderly and chaotic dynamics.