Course Title: *Chaos and Nonlinear Dynamics from Chemical, Physical and Biological Systems* [Physical Chemistry Graduate Course: offered under the official PSU title of ‘Advanced Topics in Physical Chemistry’] This course is cross-referenced as Chem 410 for those undergraduate students who might want to take the course.

Prerequisites: A general appreciation of mathematics recommended, but no special knowledge of nonlinear dynamics is required (the object of this course is to teach you nonlinear dynamics). A working knowledge of ODE’s preferable but not essential, Chem 440. The most important prerequisite is your curiosity to learn something new. A new way to look at nature and natural processes. The course will stay on topic: Is chaos universal? Is this a unifying theory underlying all (or at least, many) dynamical systems? The course intends to present the universality of chaos and chaotic behavior in a large number of diverse dynamical systems.

Instructor: **Reuben H. Simoyi** (SB2 372, phone 5-3895, rsimoyi@pdx.edu)

Office Hours: Monday, Wednesday; 2:30 - 3:30 PM (Final office hours to be set after first week of classes).

Timetable: This should either be 3 65-minute lectures MWF 10:15 AM or two 100-minute lectures per week on **Mondays and Wednesdays**. Final timetable will be set after first week of classes. These times may end up being retained, or they may be altered, depending on students’ schedules.

Venue: **To be determined**


Introduction

Preamble: Chaos theory is a field of study in mathematics, with applications in several disciplines. Its now-acknowledged range is nothing short of mind-boggling. It includes geology, microbiology, biology, economics, computer science, engineering finance (!), algorithmic trading, meteorology, philosophy, physics, politics(!), population dynamics, psychology, cardiology, and even robotics. In the laboratory, chaotic behavior has been observed in electrical circuits, lasers, oscillating chemical reactions, fluid dynamics, as well as computer models of chaotic processes. Chaos theory studies the behavior of dynamical systems that are highly sensitive to initial conditions, an effect sometimes referred to as the ‘butterfly effect’: could a butterfly, flapping its wings in Tokyo, ultimately affect the weather in New York? Small differences in initial conditions can result in widely different outcomes for chaotic systems, rendering long-term prediction impossible (such as in weather forecasting). This happens even though these systems are deterministic, in which their future behavior is fully determined by their initial conditions with no random elements involved. Thus the deterministic nature of these systems should make them predictable. This behavior is known as deterministic chaos. It is like a contradiction in terms: chaos and determinism…. but it is not.

Thus the Biblical definition of chaos does not apply here. Mathematically, chaos is defined rigorously by three strict and necessary properties. To be chaotic, a system must be (a) sensitive to initial conditions (with a finite, non-zero leading Lyapunov exponent and positive Kolmogorov-Sinai metric entropy), (b) topologically mixing (any given open set of its phase space will eventually overlap with any other given region; i.e. phase space trajectories should define a strange attractor), and (c) its periodic orbits must be dense (any point in its phase space is approached arbitrarily closely by periodic orbits). Sensitive dependence on initial conditions means that there exists a set of initial conditions of positive measure which do not converge to a cycle of any length.

The existence of chaos had been postulated in the 19th Century by the great French mathematician, Poincare', but it was Lorenz who suggested its existence in dissipative dynamical systems, starting with hydrodynamic fluid flow. Lorenz proved that chaos can exist in systems with three or more coupled ordinary differential equations. Feigenbaum also proved that chaos can exist in discrete onto mappings via the period-doubling sequence. What was most important is that simple mathematical models can generate chaotic behavior and that these simple models could be used to describe very complex real systems. Chaos is the name given to intrinsic randomness, which is random behavior arising from deterministic systems. Chemical chaos in particular has been restricted to the behavior of chemical oscillatory systems. With the help of a suitable bifurcation parameter, e.g. temperature, flow rate or concentrations, the continuous oscillatory system can be studied by applying discrete recursive formulae and symbolic dynamics.
Chaotic behavior can also be observed in many physically unrelated systems. Chaotic behavior as applied to nonlinear systems should be characterized, apart from a positive leading Lyapunov exponent, by continuous Fourier spectra and strange attractors with fractal structures/dimensions.

Chaos theory is currently being applied to medical studies of epilepsy, specifically to the prediction of seemingly random seizures by studying initial conditions. From chemistry; this course will attempt to take the student from the basic mechanistic understanding of clock reaction behavior, to the generation of complex oscillatory dynamics and the link to chaotic behavior. In physics, the RLC nonlinear electrical circuit will be studied. In biochemistry, we will study glycolytic oscillations as well as oscillations of cAMP in Dictyostelium cells. In biology, we will study circadian rhythms.

The student is allowed to take out of the course what they feel is most important to them. The second paragraph of this preamble, containing hard core mathematical analyses of chaos is unnecessary for the student who might not be so inclined. Such a student can skip completely all these aspects with absolutely no penalty while concentrating on the general dynamical systems themselves.

General Syllabus.

I

Introduction: far from equilibrium behavior, feedback loops, clock behavior, autocatalysis. Simple models, the Lotka-Volterra scheme, the Brusselator model, bistability, flow diagrams, reaction-diffusion schemes.

II

Chemical Kinetics: Mechanisms, the Belousov-Zhabotinsky reaction, stability analysis, the Jacobian, eigenvalues and eigenvectors, multivariable systems, attractors, phase diagrams, oscillatory dynamics, the FKN mechanism.

III

Experimental techniques: Systematic design of chemical oscillators, batch and flow reactors, the CSTR environment and design, (the BZ system is used as an example for most of this section).

IV

Biological oscillators: cell cycles, neural oscillators and networks, bursting.
**Modeling:** Computational tools, stiff ODE’s, semi-implicit methods, Euler, Taylor, Runge Kutta techniques. Simulating the Lorenz hydrodynamic system with three variables. Generating a strange attractor.

**VI**


**VII**

*Chaotic dynamics:* This section will deal with chemical and non-chemical systems that show chaotic dynamics. The use of ‘onto’ maps and derivation of symbolic dynamics, the RLR sequences of Metropolis, Stein and Stein (J. Comb. Theory, Ser. A; 1973) Routes to chaos and bifurcation diagrams; biological population growth; the Lorenz model for convecting fluid. Period ‘three’ means chaos.

**VIII**

*Glycolytic oscillations.* The oscillatory enzymes involved. The allosteric model for GO’s. Experiments and experimental data

**IX**

*Circadian rhythm and oscillations.* The circadian clock in the drosophila. The model for circadian oscillations in the drosophila PER protein

Each section should take 3-4 lectures. Some sections, such as IV and VIII will not be handled in too much detail so that class will spend more time on the introductory aspects of the course which are covered in sections I and II. The class needs a good base from which to build upon. There is really no true text book which will cover topics in this course to the level the professor would prefer, but the *Epstein and Pojman* book is as close as any other text, which is why it is the recommended text. Most lecture material will be pulled out of recent literature publications. Guest professors may pop up for some items listed in sections II and V.

I hope students will have a lot of fun in this course while still learning a lot. It is a very fascinating topic and one can really get lost in it. **This subject is a little like golf: once you get into it, you become addicted.**
PS
The professor wrote the following poem (Sonnet minus 10 lines!) during his stint as a postdoctoral fellow at the University of Texas after discovering the Universal Sequence (U-sequence) of Metropolis, Stein and Stein in the BZ system:

“The U-sequence is now really quite tame
With Simoyi, Wolf and Swinney, they’ve put it to shame
With an ‘R’ here and an ‘L’ here, that’s the name of the game
And if you want to reverse bifurcate, it is still all the same”
- R. Simoyi


NB: This course used to be offered every other academic year, but, of late has not been offered for quite some time. It will continue to be offered infrequently and not as regularly as before.