Physical Chemistry II (Chem 252/442)

Knowledge Base for Midterm Exam 1

1. Non-Linear Dynamics

- Criteria for deterministic Newtonian dynamics. Specific results of linear force laws.
- Non-linear positive or negative feedback effects. Examples?
- Edward Lorenz' non-linear mathematical weather model (variables, parameters,..).

2. Non-Linear Maps

- Features of Logistic-Map (LM) dynamics, profile function, fixpoints, periodic points, attractors, strange attractors, repeller points.
- "Cob web" trajectory graphs.
- Dependence of character of the iterations on the magnitude of the gain/amplification parameter μ ? Explain the plot of asymptotic intensity I_n vs. μ .
- What does "bifurcation" or multiple bifurcation mean? What are their relation to "periodic points," points of period n?
- What is the heuristic meaning of the Lyapunov exponent λ ? What is the character of LM iterations for $\lambda <$, >, = 0?

3. Complex chemical reactions

- Reaction and equilibrium constants, reaction extent?
- Stationary vs. equilibrium chemical states reached asymptotically in chemical reactions. Relation to derivatives of reaction rates, method of variation.
- Special properties of autocatalytic and self-replication reactions.
- Examples: Oscillatory chemical reactions, and predator-prey dynamics.
- Relation to non-linear maps.

4. Cellular automata

- Cellular automata: representing basic premises for evolution.
- Representation of CA evolution rules in formal logic.
- Encoding CA rules in binary, octal, decimal representation.
- Differences between CA and random walk.

Relation of CA dynamics to diffusion in crystal lattices.

5. Fractal Structures

- Self-similar geometrical properties of fractal structures.
- What makes them different from other structures?
- · Meaning of fractal dimension.
- Examples of fractal structures found in nature and civilization.

6. Probability Distributions

- Normalization and moments, mean expectation values and variances.
- Applications of binomial, normal, and Poisson probability distributions:
- Functions of random variables.
- Meaning and practical use of the Central-Limit Theorem.

7. Mathematical

- Differentiation, Taylor and other series expansions, iterations.
- Implicit functions $f^n(x)$.
- Functions of stochastic variables.
- Sets of random numbers in Excel. Sort random events into discrete bins.
 CLT
- Series expansion of the exponential $\exp(x) = \sum_{n=0}^{\infty} \frac{1}{n!} x^n$