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 $\lambda <, >, \mathbf{=0}$?

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. <u>Fractal Structures</u>
- 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. <u>Probability Distributions</u>
- 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. <u>Mathematical</u>
- 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