ACMS 40730 - Mathematical/Computational Modeling

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Class Location: 207 DeBartolo Hall
Class Schedule: Monday and Wednesday, 2:00PM - 3:15PM
Office Hours: Friday, 2:00PM - 3:00PM
Class Website: https://www3.nd.edu/~dschiava/ACMS40730_fall17.html

Course Description - The class is designed to provide a rich, example-driven experience on how to leverage abstract mathematical concepts for the solution of real word problems in the Natural Sciences, Physics and Engineering. You will be challenged to formulate *mathematical models*, i.e., abstract and typically approximate representations of the reality, capturing a fundamental relationship between certain quantities of interests. You will be asked to solve problems for various types of models, expressed through increments (continuous or discrete), scaling and power laws, defined in probability (stochastic) and inspired by adversarial games. Time permitting, systems exhibiting chaotic behavior and predator-prey systems will also be discussed. Besides reviewing the main analytical tools to investigate the properties of these models, you will write computer code and compute their numerical solutions. The intellectual challenge for this class is to learn how to appropriately formulate models from concrete examples in various fields, to understand the approximation involved and develop the computational skills needed to pose questions with these models and efficiently derive correct answers.

Course Objectives - In this class you will learn to turn real world problems into models, ask precise questions to these models and compute precise answers. By the end of the class you will be able to:

- ✓ Formulate mathematical models of various types and critically analyze their limits and associated degrees of approximation.
- ✓ Leverage the examples discussed in class to solve problems in Applied Mathematics by creating new models or by proposing improvements of existing ones.
- ✓ Write code using a high-level programming language to translate abstract models in concrete computable tasks.

Pre-requisite - ACMS 20750 or MATH 20750 or MATH 30650.

Academic Calendar - Fall Semester 2017 - Class start: 08/22. Mid-term break 10/14 - 22. Thanksgiving Holiday 11/22-26. Last class day 12/07. Reading days 12/08-10. Final examinations 12/11-15.

Textbook

- ✓ K.K. Tung, *Topics in Mathematical Modeling*, Princeton University Press, 2007.

Textbook and other references

- ✓ E.A. Bender, An introduction to Mathematical Modeling, Dover Publications, 2000.
- ✓ S. Elaydi, An introduction to Difference Equations, Springer, 2005.
- ✓ V.I. Arnold, Ordinary Differential Equations, Springer, 2006.
- ✓ M.A. Pinsky, S. Karlin, An introduction to Stochastic Modeling, Academic Press, 2011.
- ✓ M.O. Jackson, A Brief Introduction to the Basics of Game Theory, Available online.

Scared of python? - If you are unfamiliar with python, I strongly recommend you to go through the online tutorial at `http://www.scipy-lectures.org/`, specifically: 1. Getting started with Python for science, 1.1.

Python scientific computing ecosystem, 1.2. The Python language, 1.3. NumPy: creating and manipulating numerical data and 1.4. Matplotlib: plotting. A review on these topics will however be given in the second class meeting and the first homework will allow you to familiarize with the language.

Attendance - No explicit attendance record will be kept for this class. However, the instructor may require everyone to write down questions on a form during a class meeting for a specific topic. Every question form not returned will be graded as follows: Two forms not returned: A, three: B+, four: B, five: B-, six or more: C. I hope this also stimulate interaction in class and helps to develop the priceless ability to always have questions to ask.

Required Work and Grading Criteria - The required work consists of homework problems, midterm exam, and final exam. The breakdown of marks is:

- ✓ **Attendance and participation in class:** 10%.
- ✓ **Homeworks:** 30%.
- ✓ **Midterm:** 30%.
- ✓ **Final:** 30%.

Homework Assignments - Homework assignments will be based on the material presented in class. Most of the homeworks will require to solve problems, answer questions from the theory or to develop python code. Weekly homework assignments will be made available (either in class or through the course website) on Wednesday and are expected to be returned by Monday of the following week.

Midterm Exam - An in-class 75 minutes closed-book (paper, pencils, and non-programmable calculator only) midterm exam is scheduled for **Wednesday October 11th, 2:00PM - 3:15PM**.

Final Exam - A closed-book (paper, pencils, and non-programmable calculator only) final exam will take place on **Monday, December 11th, 4:15PM - 6:15PM**.

Honor Code - All students must familiarize themselves with the Honor Code on the University's website and pledge to observe its provisions in all written and oral work, including oral presentations, quizzes and exams, and drafts and final versions of essays. While discussion in small groups in doing homework is permitted (and strongly encouraged) in this course, **the work should be your own**. Exams are closed book and are to be done completely by yourself with no help from others.

Tentative program

Week n.	From/To	Tentative Content
Week 1	Aug 22nd - Aug 25th	**Intro on modeling**. Introduction to mathematical/computational modeling. Models and reality. Properties of models. Building a model. A motivating example: long term growth of a population.
Week 2	Aug 28th - Sept 1st	**Programming**. Python tutorial. **Intro on modeling**. Improving the model. Variable growth ratio and time lags effects. Demographic models.
Week 3	Sept 4th - Sept 8th	**Difference Equations**. Motivation. Fibonacci sequence. Golden ratio. First order difference equations. Orbit, autonomous/non-autonomous equations. Solution formulae for linear first-order difference equations. Equations with constant coefficients. Example: Equilibrium amount of drug in the body. Example: amortization.
Week 4	Sept 11th - Sept 15th	**Difference Equations**. Equilibrium points and fixed point equations. Stable, asymptotically stable, unstable and attracting equilibrium points. Graphical iteration and cobweb diagrams. Cobweb phenomenon in economics. Three theorems to compute the stability of difference equations. Periodic points and cycles.

Week n.	From/To	Tentative Content
Week 5	Sept 18th - Sept 22nd	**Scaling laws**. Example: Predicting the mass-metabolic rate relation in organisms. Self-similar branching vascular networks. Area preserving principle. Volume filling principle. Example: Cost of packaging. Example: speed of racing shells. **Dimensional analysis**. Basic physical units. Dimensionally homogeneous equations. Buckingham pi theorem. Example: law of gravitation.
Week 6	Sept 25th - Sept 29th	**Differential Equations**. First-order and second-order ODEs. Existence of unique solutions. Homogeneous equations. Homogeneous and inhomogeneous superposition with examples. Variable separable equations.
Week 7	Oct 2nd - Oct 6th	**Differential Equations**. Radiometric dating. Exponential decay. Half-life. Example: age of uranium in our solar system. Example: estimating the age of the universe. Example: carbon dating. Example: HIV virus production modeling.
Week 8	Oct 9th - Oct 13th	**Models with calculus**. Kepler laws for the orbits of planets. Vector calculus, position, velocity, acceleration in polar coordinates. Rederivation of Newton gravitation law. **Phase plane analysis**. Logistic population growth models. Exact solution with variables separable. Stability. Models with harvest. Stability and maximum fishing effort. Optimal effort for maximum yield. Economic considerations. Depensation growth models.
		Midterm
Week 9	Oct 23rd - Oct 27th	**Numerical solution of ODEs**. Approximation of derivatives via Taylor expansion. Forward finite difference approximation. Order of approximation. Backward finite difference. Central differences. Finite difference schemes for second derivatives. Model problem. Forward Euler scheme. Consistency and Stability. Backward Euler scheme. Crank-Nicolson scheme. Higher order methods: Runge-Kutta schemes. Example: an implicit central difference scheme for structural dynamics.
Week 10	Oct 30th - Nov 3rd	**Stability of nonlinear ODEs**. Change of reference frame. Linearization. Determinant equation. Saddle point. Stable/unstable node. Stable/unstable focus. Center. Graphical representation using invariants. **Predator-prey systems**. Lotka-Volterra models and predator-prey systems. Linear stability at zero population. Oscillating linearized solution for finite population equilibria. Periodicity of nonlinear solutions in the population plane. Average of periodic solutions. Equations with harvest.
Week 11	Nov 6th - Nov 10th	**Compartmental models**. SIR model and graphical formulation in terms of compartments and fluxes. Epidemic conditions. Numerical simulation of SIR models. **Chaotic models**. Properties of chaotic systems. Forward Euler solution of logistic population growth model. Time step selection. Numerical simulation at increasing time steps and demonstration of chaos. Chaos in deterministic differential systems. Conditions for chaos in ODEs. Lorenz equations for thermal convection. Equilibrium points and linearized equations.

Week n.	From/To	Tentative Content
Week 12	Nov 13th - Nov 17th	**Chaotic models**. Transition between stable and unstable behavior and selection of parameters leading to chaos. Numerical simulation of the Lorenz equations. **Stochastic modeling**. Events. Probability of events and properties. Addition law, law of total probability. Random variables and distribution function. Continuous and discrete random variables. Moments and expected values. Conditional probabilities. Example: urns with gold and silver coins. Stochastic processes and Markov chains. Markov property and one-step transition probability matrix. Probability of transition in multiple steps.
Week 13	Nov 20th	**Stochastic modeling**. Example: weather forecast from one week of data. Computing probabilities through Markov models. General Markov chain with absorption. Simulating Markov chains. Projections on the inverse distribution function. Algorithm for random transitions and Python implementation.
Week 14	Nov 27th - Dec 1st	**Stochastic modeling**. Example: taxicab stand, states and one-step transition probabilities. Intuition on its long run behavior. Regular Markov chains and limiting distribution. Example: long run behavior of a two-state Markov chain. Computing the limiting distribution by solving a linear system of equations with examples.
Week 15	Dec 4th - Dec 8th	**Game theory**. Intro on non-cooperative games. Games in normal form. Dominant strategies. Examples: prisoner's dilemma and Cournot duopoly. Nash equilibria. Examples: two-firms advertisement problem, hawk/dove and chicken games. **Pre-final review**.