ABE 5646-4162
Course Overview & Introduction to Systems Analysis Concepts
Frazier-Rogers Hall Room 283

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Objectives

1) To learn to basic modeling and simulation methods for biological and agricultural systems
   • Systems Approach
   • Model development
   • Example models
   • Numerical Simulation

2) To learn methods for working with dynamic models
   • Model evaluation
   • Sensitivity analysis
   • Parameter estimation
   • Applications
Overall Format

The course will contain two components. For about the first 1/3 of the course, students will be exposed to basic concepts of systems analysis, modeling and computer simulation of agricultural and biological systems. Emphasis will be placed on continuous simulation of dynamic models with examples that give students a broad exposure to dynamic models. Most of the reading material for this part of the course will be made available by the instructor via the course web site. Much of the basic information will be from the book by Keen and Spain (1992), which is now out of print. Students will also be referred to a new book for examples of biological models: Datta, A.K. and V. Rakesh. 2010. *An Introduction to Modeling of Transport Processes: Applications to Biomedical Systems*. Cambridge University Press.

The second part of the course will introduce students to various methods for working with dynamic models, starting with sensitivity analysis, going into parameter estimation and model evaluation. An overview of applications of models in agricultural and biological systems will be given. The text for this part of the course is the book by Wallach et al. (2006) entitled “Working with Dynamic Crop Models: Evaluation, Analysis, Parameterization, and Applications”. During this part of the class, students will also be exposed to uncertainties in models associated with uncertainties in model parameters, inputs, and structure.
<table>
<thead>
<tr>
<th>Week</th>
<th>Description</th>
<th>Reading Material</th>
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<tbody>
<tr>
<td>1</td>
<td>Course Overview</td>
<td>Jones &amp; Luyten (1998)</td>
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<tr>
<td></td>
<td>Introduction to Systems</td>
<td></td>
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<td></td>
<td>Diagrams used in Systems Analysis</td>
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<td>Modeling Concepts</td>
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<td></td>
<td>Forrestor Diagram Conceptual Model, Example Model</td>
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<td></td>
<td>Assumptions in Model Development</td>
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<td></td>
<td>Finite Difference, continuous states, discrete time</td>
<td>Keen &amp; Spain (1992) Ch 5</td>
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<td>Simple Methods</td>
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<td>Euler</td>
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<td>Trapezoid</td>
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<td>Runge-Kutta</td>
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<td>Choice of time step</td>
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<td>Errors in Numerical Simulation</td>
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## Outline

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<thead>
<tr>
<th>Week</th>
<th>Description</th>
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<tbody>
<tr>
<td>3</td>
<td>Back to Modeling – Biological &amp; Physical Models</td>
<td>Keen &amp; Spain (1992) Ch. 1-2, 6-8</td>
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<tr>
<td></td>
<td>• Growth</td>
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<td></td>
<td>• Heat flow and temperature</td>
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<td>• Passive Diffusion</td>
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<td></td>
<td>• Inhibited growth</td>
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<td>• Michaelis-Menten model of enzyme reactions</td>
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<td>• Kinetics of biochemical reactions</td>
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<td>• Homogenous Population of organisms</td>
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<td>• Chemostat microbial growth (batch, continuous flow)</td>
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<td>4</td>
<td>Additional Modeling Concepts</td>
<td>Keen &amp; Spain (1992) Ch. 7, 9, 13, 14</td>
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<td></td>
<td>• Compartment models of biogeochemical systems</td>
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<td>• Lags in dynamic biological models</td>
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<td>• Adding an age dimension in biological models</td>
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<td>• Adding spatial dimensions in dynamic models</td>
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<td>Week</td>
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| 5    | Modeling Temperature Effects on Biological Systems  
      • Effects on chemical reaction rates  
      • Effects on biological activity, general  
      • Effects on developmental processes in plants and other biological organisms  
      • Degree-day models: basis for and use of | Keen & Spain (1992) Ch. 12  
Handout; degree-days |
| 6    | Crop Modeling  
      • State variables  
      • Development  
      • Dry matter growth  
      - photosynthesis, respiration  
      - Light Use Efficiency (LUE)  
      • Partitioning of dry matter | Jones & Luyten (1998)  
Salazar Papers on Node development & on Growth  
Wallach et al. (2006) Chapter 9  
Jones et al. (2003) |
| 7    | **Mid Term Exam** | --- |
|      | Introduction to Working with Dynamic <crop> Models  
Two forms of <crop> models | Wallach et al. (2006) Ch 1 |
# Outline

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<tr>
<th>Week</th>
<th>Description</th>
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<tbody>
<tr>
<td>8</td>
<td>Review of Basic Statistics, Random Variables</td>
<td>Wallach et al. (2006) Ch 1, Appendix Other References</td>
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<tr>
<td></td>
<td>Why these are important in simulation</td>
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<td>Examples</td>
<td></td>
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<td></td>
<td>Distributions</td>
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<td>Expectation</td>
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<td></td>
<td>Working with Statistics in Simulation</td>
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<td>Approximation of distributions from numerical outputs</td>
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<td>Expected Values (Mean, Variance, Covariance – 2 methods)</td>
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<td>Random Sampling, Monte Carlo Methods</td>
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<td>Bayesian Statistics</td>
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<td>9</td>
<td>Introduction to the R Programming environment, with exercises</td>
<td>Handout</td>
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<td>10</td>
<td>Spring Break (March 5-12)</td>
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<td></td>
<td>• Comparing a model with data</td>
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<td>• Graphical, errors</td>
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<td>• Measures of agreement (bias in mean, variance)</td>
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<td>• Evaluation of predictive quality</td>
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<td>• Cross validation</td>
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<td>• Bootstrap estimation</td>
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<th>Week</th>
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| 12   | Uncertainty and Sensitivity Analysis  
  • Uncertainty of parameters, inputs  
  • Model output analysis, probability distributions  
  • Local sensitivity analysis (absolute, relative)  
  • Global Sensitivity Analysis  
    - Monte Carlo sampling  
    - Analysis of output variance (ANOVA) | Wallach et al. (2006)  
  Ch 3  
  Jones Handout |
| 13   | Parameter Estimation  
  • Least Squares (non-linear)  
  • Choice of parameters  
  • Multiple variable observations  
  • Monte Carlo methods  
    - Metropolis-Hastings  
    - GLUE  
    - Parameter uncertainty and correlation | Wallach et al. (2006)  
  Ch 4 |
| 14   | Optimization with Simulation Models  
  Data Assimilation with Dynamic Models | Wallach et al. (2006)  
  Ch 5, 6 |
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<th>Week</th>
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<tbody>
<tr>
<td>15-16</td>
<td>Special Project Presentations</td>
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<td>Apr 19</td>
<td>Review for Final Exam</td>
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<tr>
<td>Apr 20</td>
<td>Last Day of Classes</td>
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<td>Apr 20</td>
<td>Final Project Reports due on or before this date</td>
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<td>Tuesday, Apr 26, 12:30 – 2:30 pm</td>
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<td>Final Exam - ABE 5646 (Exam 26C)</td>
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<td>ROG 283</td>
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Grading

- Homework 30%
- Mid-term Exam 20%
- Final Exam 20%
- Project 30%
Class Lectures

Lectures will be held on Tuesday during class periods 2 and 3 (8:30 – 10:25 am) and on Thursday during class period 2 (8:30 – 9:20 am). The additional class period allocated for the course (period 3 on Thursdays) will be used as needed for presenting additional material or for discussions and reviews.
Textbook and other Reading Material

TEXTBOOK


HANDOUTS will include pages from:

Other Reading Material

Introduction to Systems Analysis

• Terminology
• Systems Diagrams
• Dynamic Models and Modeling
• Systems Analysis Approach
• Dynamic Models
• Forrestor Diagrams
• Example system, diagram, equations
Some Perspectives of Systems Approach in Agricultural and Biological/Ecological Systems
Information Needs in a Systems Approach

- Agricultural Science is not a science unless it predicts and tests its predictions (P. G. Cox, 1996)

- Understanding $\rightarrow$ Prediction $\rightarrow$ Control, Manage (H. Nix, 1983)

- A wealth of research information exists concerning the possibilities for change, the options available and the likely effects of a range of land use practices. However, it is less clear how this information is of use to, or can be filtered into, decision making processes. (J. Park and R. A. F. Seaton, 1996)
Systems Approach

**Research for Understanding**
- Research
- Increased Understanding
- Model Development

**Problem Solving**
- Model
- Prediction
- Test Predictions
- Application/Analysis
- Control/Management/Decision Support
Systems Approach for Research and Applications

- Resource inventory
- Research
- Database
- Simulation models
- Expert systems
- Predictions
- Prescriptions
- Validation
- Calibration
- Strategic & tactical applications

— G. Uehara
Incorporating Crop Models into Traditional Agronomic Research

Question, Problem

Hypotheses

Experiments

Analysis

Conclusions, Decisions

Recommendations
Hierarchy is Important in Biological/Ecological/Agricultural Systems

- **WORLD**
- **REGIONS**
- **FARMING AREAS**
  - CROP ECOSYSTEMS
    - CORN, PASTURE, ...
  - ELEMENTS
    - INDIVIDUAL PLANTS, ...
  - COMPONENTS
    - LEAVES, STEMS, ROOTS, ...
- **MICRO-COMPONENTS**
  - STOMATA, BIO-CHEM. PATHWAYS...
Terminology (Jones & Luyten, 1998)

- **System**: a collection of components and their interrelationships that have been grouped together for the purpose of studying some part of the real world
  - Biological systems tend to hierarchically organized and can be studied at a number of levels
- **Environment**: everything except the components of the system
- **System Boundary**: abstraction of the limits of the system components, separating them from the environment
- **Model**: a mathematical representation of a system
- **Modeling**: process of developing the representation of a system
- **Computer Simulation**: includes processes necessary for operationalizing or solving a model to mimic real system behavior
  - Developing computer logic and flow diagrams, writing the computer code and implementing the code on a computer are tasks
Terminology (Jones & Luyten, 1998)

- **Inputs:** factors in the environment that influence the behavior of the system but are not influenced by the system
  - (Exogenous variables, driving variables, forcing functions)
  - May vary with time (rainfall, temperature, light, tide, etc…)

- **Outputs:** represent the characteristic behavior of the system that is of interest to the modeler (crop biomass, yield, meHg concentration)

- **Parameters and Constants:** characteristics of the components of the model that are constant through simulated time
  - Constants - Molecular weight of glucose, gravitational constant, number of seconds in a day, days in January
  - Parameters – daily caloric requirement, water use efficiency, soil water resistance, respiration loss
System Diagrams

- Help analysts design a model
- Communicate model structure, components to others
- Show relationships among components
- Help analysts organize concepts, assumptions
- Help in development of mathematical model
- There are different diagram types
Dynamic Models

- Play important role in systems analysis
- Derived from understanding of system
- Physical, biological, economic
- Simplification of reality
  - “All models are wrong, but some are useful”
    G. E. P. Box quote
- General form -
  \[
  \frac{dX(t)}{dt} = f \{X(t), u(t), p\}
  \]
Terminology (Jones & Luyten, 1998)

- **State Variables**: quantities that describe the conditions of system components
  - Change with time in dynamic models as system components interact with each other and the environment
  - Soil water content, crop biomass, elephant happiness…

- **Process Model**: interrelationships between components in a system, and therefore between state variables in the system, exist because of various processes
  - **Continuous models**: characterized by state variables that can change smoothly over small time intervals and are not restricted to integers
  - **Discrete models**: characterized by state variables that can change in integers over time intervals (# of live births), populations etc…
Terminology (Jones & Luyten, 1998)

- **Verification**: the evaluation of the accuracy with which the computer code represents the mathematical model and the programmer's intentions
  - Checking of mathematics, units, programming logic and code errors
  - Does the model work like I expect it to?

- **Calibration**: making adjustments to the model parameters to give the best fit between simulated results and results obtained from measurements

- **Validation**: process of comparing simulated results to real system data not previously used in any calibration or parameter estimation process.
  - Is the model sufficiently accurate for its application?
  - As defined by objectives of the simulation study
Systems Approach

• Statement of Objectives
  – Critical step, often overlooked
  – What to develop? Who are the users?
  – Better understanding? vs. Solving the problem?

• Definition of the System
  – System boundary, inputs, outputs

• Literature Review and Data Analysis

• Model Development (Design, Code, Parameters)

• Sensitivity Analysis

• Model Accuracy Evaluation (gaining confidence in the model)

• Model Application
Cropping System Diagram
Modeling

- Continuous systems modeling is a process-oriented approach for describing system behavior.
- Three types of processes:
  - Transport
  - Transformation
  - Storage
- Processes are described by two types of variables:
  - Extensive (storage & flow-through quantities, i.e. mass, volume, heat, money)
  - Intensive (represent the driving forces for the extensive variables, i.e., force, pressure, temperature, etc.)
- Example: heat flow through a wall is described by its heat conduction (extensive) and the temperature differential (intensive).
- Extensive variables are measured at a point, intensive variables are measured across an object.
- In biological systems, these are hard to determine!
  - Complex states or storage quantities
  - Scale of model may prevent the use of a real intensive variable, leading to empirical descriptions of flow rates.
Modeling continued

• Compartment Models
  – Primary emphasis on flows and storages of system variables
  – First order differential equations can be derived from compartment structure

• Forrester (1961) is most commonly used diagramming system

\[
\frac{dX_i}{dt} = \sum_j I_{i,j} - \sum_k O_{i,k}
\]

\(i.e.\) Change in level per unit time = Sum of Flow Rates into compartment \(i\) minus Sum of Flow Rates out of compartment \(i\)
Forrester Diagrams (1961)

- **a)** Level
- **b)** Rate
- **c)** Source
- **d)** Auxiliary Variable
- **e)** Pathway for material
- **f)** Pathway for information flow
Two Water Tank Example

\[ V_1 = A_1 \times H_1 \]

\[ V_2 = A_2 \times H_2 \]
System
2 Storage Compartments
\((i = 2)\)
3 Flows
\((j = 3)\)

\[
\frac{dV_i}{dt} = \sum_j I_{i,j} - \sum_k O_{i,k}
\]
\[ \frac{dV_1}{dt} = i(t) - f_{1,2}(t) \]

\[ f_{1,2}(t) = C_1 \sqrt{2gH_1} \]

\[ \frac{dV_2}{dt} = f_{1,2}(t) - O(t) \]

\[ O(t) = C_2 \sqrt{2gH_2} \]
Two Water Tank Example

\[ \frac{dV_1}{dt} = i(t) - f_{1,2}(t) \]

\[ f_{1,2}(t) = C_1 \sqrt{2gH_1} \]

\[ \frac{dV_2}{dt} = f_{1,2}(t) - O(t) \]

\[ O(t) = C_2 \sqrt{2gH_2} \]
Two Water Tank Example

substituting $H_i = V_i/A_i$ for each tank

\[
\frac{dV_1}{dt} = i(t) - C_1 \sqrt{2g \frac{V_1}{A_1}}
\]

\[
\frac{dV_2}{dt} = C_1 \sqrt{2g \frac{V_1}{A_1}} - C_2 \sqrt{2g \frac{V_2}{A_2}}
\]
Two Water Tank Example Equations

\[
\frac{dV_1}{dt} = i(t) - C_1 \sqrt{2g \frac{V_1}{A_1}}
\]

\[
\frac{dV_2}{dt} = f_{1,2}(t) - C_2 \sqrt{2g \frac{V_2}{A_2}}
\]

Standard Forrester Form

\[
\frac{dX_i}{dt} = \sum_j I_{i,j} - \sum_k O_{i,k}
\]

General Functional Form

\[
\frac{dX(t)}{dt} = f\{X(t), u(t), p}\}
\]
Some Key Points

• Assumptions about compartments
• Assumptions about rates
• Rate equations – based on physics, chemistry laws or empirical
• Two compartments led to two equations and two state variables
• Could have many flows, but state variable number always equals the number of storage compartments
Complexity of System Models

- Modeling approach (diagrams, mathematical representation as first order differential equations, numerical solution/simulation) works with simple to complex models
- What characterizes a simple vs. complex system model?
- What are some difficulties associated with this approach?
Systems Dynamics Software!

- **Commercial Tools**

- **Free Tools**
  - The R programming Language
  - VisSim
  - Mapsys:
  - Consideo
  - Netlogo: (agent-based simulation)
    - [http://ccl.northwestern.edu/netlogo/](http://ccl.northwestern.edu/netlogo/)
Introduction to Systems Approach and Modeling in Agricultural & Biological Systems