Scientific Simulation and Modeling

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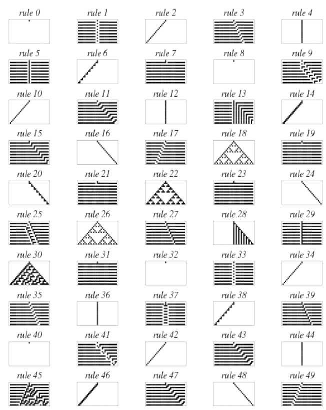
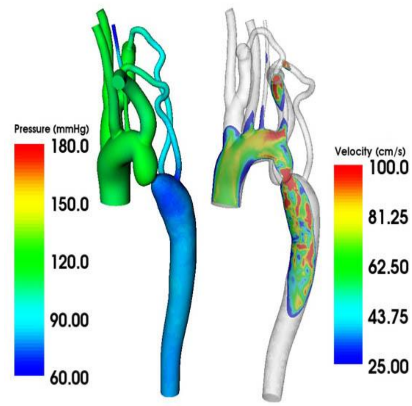
Simulation and modeling is an emerging "third leg" of scientific investigation. Like experimentation and theory, simulation provides a means to investigate and test hypotheses about the natural world. Unlike experimentation and theory, however, simulation is still a formative methodology. Successful simulations incorporate elements of theoretical models and experimental findings.





This class is meant to be a broad survey of different modeling and simulation techniques as applied to scientific and engineering domains. However, it will also be participation-intensive, as class presentations and projects will constitute a majority of the final grade.

Assignments	Item	Final Grade Total
Homework #1	Software Package Review	15%
Exam #1	Module #1	20%
Exam#2	Module #2	20%
Homework #2	Model type review and proposal	15%
Project	Group presentations	15%
	Write-up	15%

There will be two exams, two homework assignments, and a group project. The group project will consist of like-minded individuals picking a problem, a software platform, and producing a small-scale test of the idea. Homework assignments #1 and #2 will contribute to the final project, as you will be asked to review different software packages and come up with ways to test hypotheses with them. Ideally, Homework #2 will arise from your initial interactions with group members (i.e. each member will champion a certain idea to test, with the project involving the implementation of one or two of these ideas). While I have provided several reference books listed after each section of Module #2 to give you project ideas, please do not limit your scope to these examples. The goal here is to come up with something useful (and fun!).

Module #1: Introduction to Computational Modeling

Section #1: Key terms and concepts

Introductory session. Handout will be provided, use it study for first exam.

Section #2: Software package review and project group formation

Homework #1 (15% of grade) - A short (5-7 minutes) review of a specialized software package of your choosing (must be relevant to model-building or simulation). Examples include:

* SimTK (http://www.simtk.org)

* NetLogo (http://ccl.northwestern.edu/netlogo/)

* Avida (http://devolab.cse.msu.edu/software/avida/)

* breve (http://www.spiderland.org/)

A successful (i.e. 100%) presentation will include the following:

* Brief description of the package (what is does, how it works)

* How useful it is (what the package can or can't do when compared to the real world)

Exam #1 (20% of grade) - Exam will cover key terms, concepts, and software packages.

Module #2: Examples from different types of models

Section #1: Virtual environments

Virtual environments, popularized in movies such as *The Lawnmower Man* and *The Matrix*, are actually useful tools for scientific and engineering research. While many of the early developments were largely based on visual simulation, modern technologies include haptic and sensor-based I/O devices. In this section, we will focus on applications of virtual environments to tele- and neuro-rehabilitation technologies, which assist patients in recovering from stroke and balance problems.

Reference Books:
Stanney, K.M. (2002). Handbook of Virtual Environments: Design, Implementation, and Applications. CRC Press.

Magnenat-Thalmann, N. and Thalmann, D. (2004). Handbook of Virtual Humans, Wiley and Sons.

Westwood, J.D., H. M. Hoffman, H.M., and Mogel, G.T. (2002). Medicine Meets Virtual Reality, IOS Press.

Section #2: Evolutionary simulations, genetic algorithms

Evolution is perhaps the most amazing feat of nature. Life can adapt to acquire many specialized traits and functions. Harnessing this awesome power has been the goal of evolutionary simulation for several decades. We will cover issues related to artificial life, evolutionary algorithms, and mathematical modeling. If time permits, we may discuss bioinformatic approaches.

Reference Books:
Goldberg, D.E. (1989). Genetic Algorithms in Search, Optimization, and Machine Learning, Addison-Wesley.

Holland, J.H. (1992). Adaptation in Natural and Artificial Systems: An Introductory Analysis with Applications to Biology, Control, and Artificial Intelligence, MIT Press.

Nowak, M.A. (2006). Evolutionary Dynamics: Exploring the Equations of Life, Belknap Press.

Wagner, A. (2007). Robustness and Evolvability in Living Systems, Princeton Press.

Section #3: Biologically-inspired models and Physics-based simulations

Evolution has also provided us with a range of "natural" designs: objects such as Gecko's feet and virus capsids have proven to be extremely durable, functional, and elegant. Along with the need for innovation comes the need to harness the elegance of these designs for technological purposes, since evolution is a several-billion year old iterative design process. In light of this, we will discuss evolutionary dynamics and focus on examples from nature.

Reference Books:
Bar-Cohen, Y. (2005). Biomimetics: biologically-inspired technology, CRC Press.

Vogel, S. and K.K. Davis (1993). Cats' Paws and Catapults: Mechanical Worlds of Nature and People, W.W. Norton.

Vogel, S. and Calvert, R.A. (1993). Vital Circuits: On Pumps, Pipes, and the Workings of Circulatory Systems, Oxford Press.

Section #4: Complex networks, cellular automata, and excitable media

Bornholdt, S. and Schuster, H.G. (2003). Handbook of Graphs and Networks: From the Genome to the Internet, Wiley-VCH.

Csermely, P. (2006). Weak Links: Stabilizers of Complex Systems from Proteins to Social Networks, Springer.

Winfree, A.T. (1987). When Time Breaks Down: The Three-Dimensional Dynamics of Electrochemical Waves and Cardiac Arrhythmias, Princeton Press.

Wolfram, S. (2002). A New Kind of Science, Wolfram Media.

Strogatz, S. (2004). Sync: The Emerging Science of Spontaneous Order, Hyperion.

Section #4: Agent-based models

The interaction of agents or individual elements in groups is a "hard" problem, but one which we can model using relatively simple techniques. We will discuss the basic premise of this type of modeling and how it can be used for scientific and engineering purposes.

Reference Books:
Axelrod, R. (1997). The Complexity of Cooperation: Agent-Based Models of Competition and Collaboration, Princeton Press.

Bonabeau, E., Dorigo, M., Theraulaz, G. (1999). Swarm Intelligence: From Natural to Artificial Systems, Oxford Press.

Zhang, Z. and Zhang, C. (2004). Agent-Based Hybrid Intelligent Systems, Springer.

Exam #2 (20% of grade) - Exam will cover key ideas and problems sets based on each model type.

Module #3: Applying models to real-world settings

Section #1: Application domains

Homework #2 (15% of grade) - pick a model type, report on one technical aspect/challenge, propose an experiment using model to solve a real-world problem.

Section #2: Future applications

Module #4: project presentations

Presentation (15% of grade) - all group members must work together on this. It is generally best to assign non-essential tasks to specific members of the group, that way there is no ambiguity as to who didn't contribute but the project still gets done. Each group will have 30 minutes to describe the problem, describe their solution approach, present the results, and communicate the implications of and future steps in this work.

Write-up (15% of grade) - again, all group members must work together on this. One person will be responsible for communicating to me any problems and submitting both the presentation slides and report. I have ways of detecting plagiarism and cheating, so don’t try it.
The write-up will be due at the beginning of finals week.