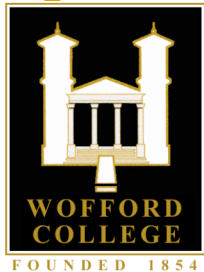


Reaching Out to Science Students
with
Computational Science and Modeling

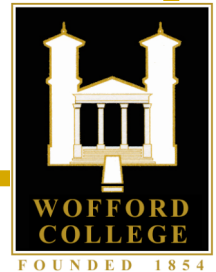
Angela Shiflet, Ph. D.
Wofford College

AAPT Topical Conference:
Computational Physics for Upper-Level Physics Programs

July 28, 2007



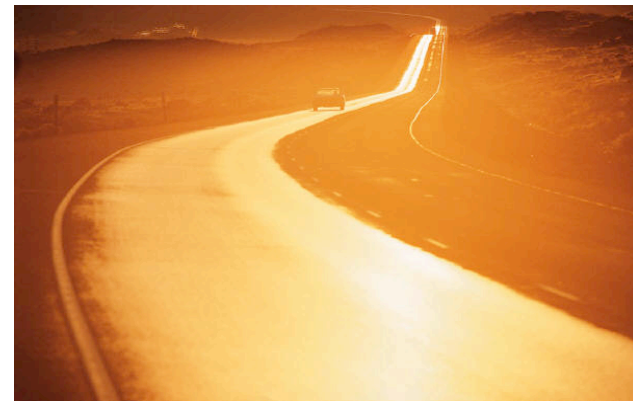
<http://www.wofford.edu/ecs/>





Overview

- Undergraduate computational science and engineering
 - Recommendations
 - Wofford's Emphasis
 - Content areas
 - Internships
 - Applications
- Questions





A SIAM Working Group Report

- Undergraduate Computational Science and Engineering Education
- Sponsored by SIAM Education Committee
- Working Group Members
 - Peter Turner (Clarkson University, Chair)
 - Kirk Jordan (IBM)
 - Linda Petzold (UC Santa Barbara)
 - Angela Shiflet (Wofford College)
 - Ignatios Vakalis (Capital University, OH)

<http://www.wofford.edu/ecs/>



Common Curriculum Content Components (1)

- Simulation and Modeling
- Programming and algorithms
 - A high level language, elementary data structures, analysis
- Applied mathematics
 - Calculus and differential equations, linear algebra, (discrete) dynamical systems
- Numerical methods
 - Errors, nonlinear equations, solving systems of linear equations, interpolation and curve fitting, optimization, Monte Carlo, ODEs, PDEs
- Parallel programming
- Scientific visualization



Common Curriculum Content Components (2)

- Application domain content
 - At least one major application area of science or engineering
- Team-based projects
- Effective technical analysis and presentation
- Research or Professional Experience
 - Independent research, presentation of solution methodologies, internship



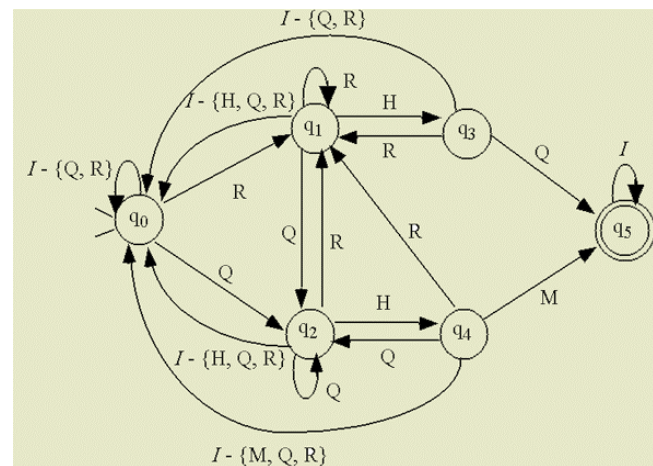
Wofford's Emphasis in Computational Science (ECS)

- Bachelor of Science
- 5 courses
 - Programming
 - Data Structures
 - Calculus I
 - Data and Visualization
 - Modeling and Simulation
- Summer internship involving computation in the sciences



Content Area: Programming & Algorithms

- Examples
 - Genomic Sequence Comparison
 - Music
 - Space

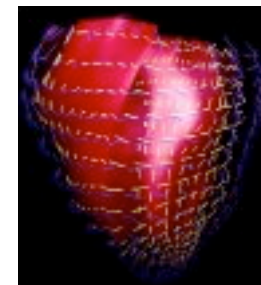




Internship: Programming



- Department of Bioengineering, U. of California, San Diego
- Multiscale computational models of cardiac electrical activity and validating them with experimental data
 - Efficiency testing and analysis
 - Changed direction of lab's research
- Medical school





Internship: Programming



- Extensible Framework for the Mathematical Manipulation Of Music
- *Mathematica*
- Fullerton Foundation Community of Scholars at Wofford
- U. OK graduate school in theoretical physics

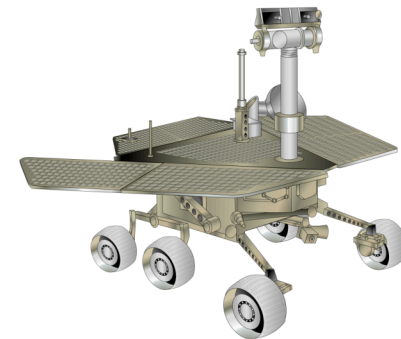
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Internship: Programming



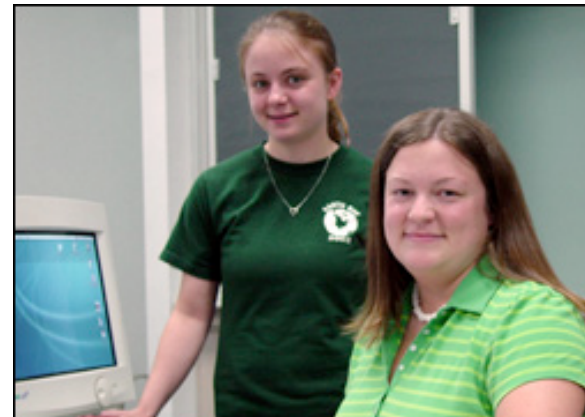
- Jet Propulsion Laboratory
- Software for Mars Rover Operations
- NSF Graduate Research Fellowship
 - Computer Graphics Laboratory at Columbia U. in New York
 - Physics, applied math & CS
 - Cloth simulation
 - Disney Studios internship





Data and Visualization: Web Assessable Databases

- UNIX
- Accessing and creating databases with SQL
- Creating web forms, HTML
- Interfacing, Perl
- Teams





Excitement to Experience to Expertise



- Genetic epidemiology at Greenwood Genetic Center
- Developed Perl program to automate linkage analysis on disease genes
- Created database on diets of Honduran women
- Used SAS (Statistical Analysis System) to examine relationship between diet and birth defects



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Excitement to Experience to Expertise



- Massachusetts General Hospital/Harvard
- National Institutes of Health
- NIH research fellowship, then graduate school in genetics
 - Finding genetic associations with obesity
 - Perl programs
 - Database to store our genotypes
 - Work with many software programs

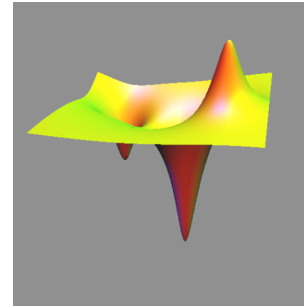


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Data and Visualization: Scientific Visualization

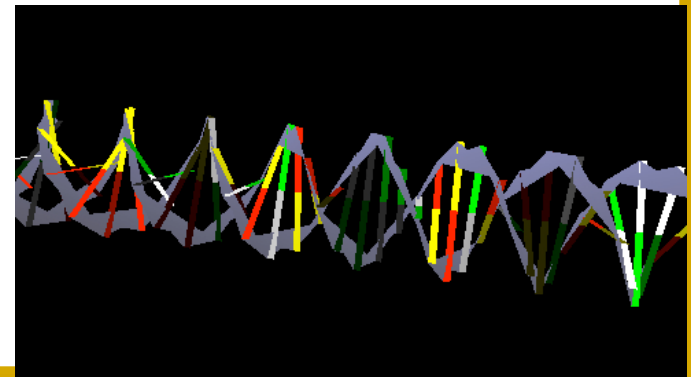
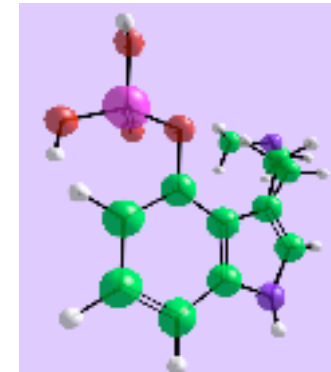
- Science examples involving 3D interactive computer animations



- C and OpenGL
- *Computer Graphics: Programming, Problem Solving, and Visual Communication* by Steve Cunningham, Prentice Hall, 2007
 - www.cs.csustan.edu/~rsc/NSF

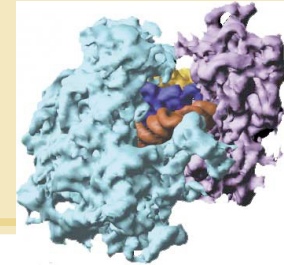
Visualization Applications

- DNA and other molecules
- Movement of ocean waves
- Diffusion across membrane
- Heat diffusion
- Spread of disease
- Lorenz equations





Internship: Medical Imaging



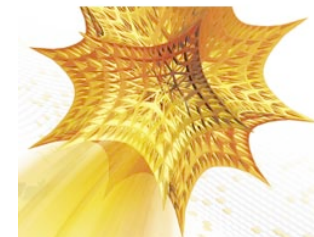
- Howard Hughes Medical Institute at the Wadsworth Center, NY Dept. of Health
- Cryo-Electron Microscopy and 3D Computer Image Processing on Ribosome
- To study structure & mechanism of protein synthesis
- National Center for Biotechnology in Madrid
- CSE '07

<http://www.wofford.edu/ecs/>



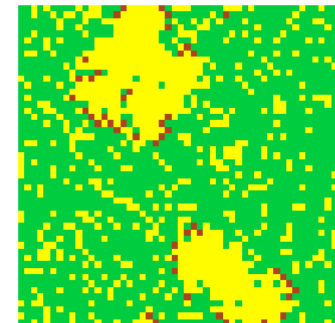
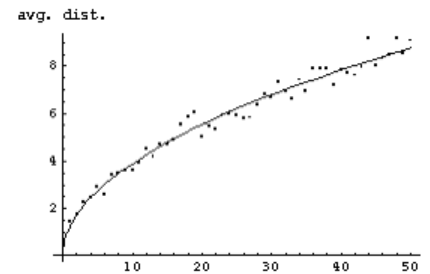
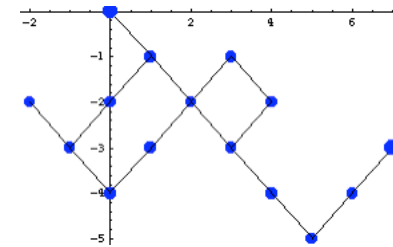
Modeling and Simulation

- No prerequisites
- System dynamics models
 - Global view
 - Differential/difference equations
- Cellular automata simulations
 - Local view
 - Stochastic
 - *Mathematica, Maple, MATLAB, Excel,* programming languages



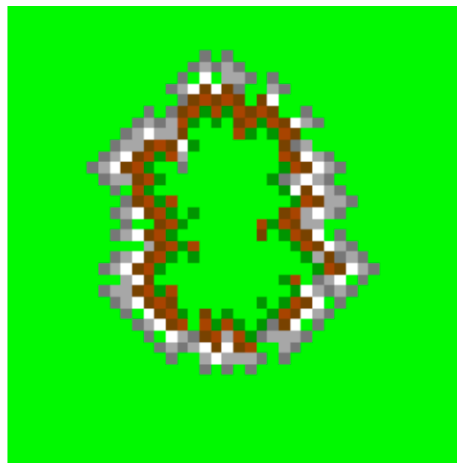
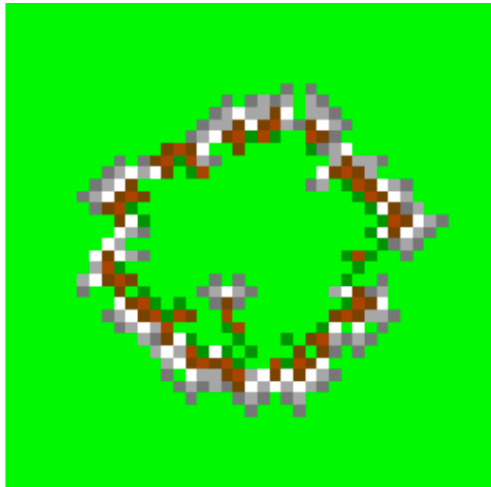
Modeling and Simulation: Cellular Automata Applications

- Brownian motion
- Movement of ants
- Spread of fire
- HIV in body
- Foraging behavior
- Spread of disease
- Fish schooling
- Pit vipers and heat diffusion
- Snow flakes - solidification





Modeling and Simulation: Mushroom fairy rings



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Modeling and Simulation: System Dynamics Tools

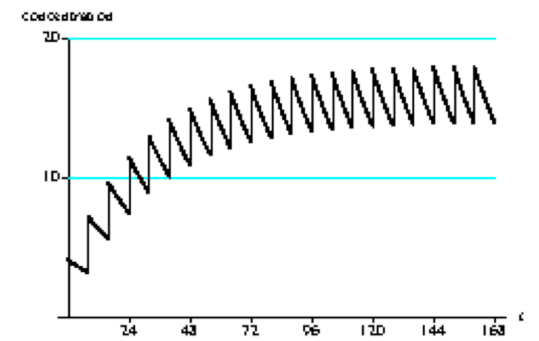
- Dynamic systems usually
 - Very complex
 - Many components
 - Involved relationships
- Tool can lower mathematical barriers
 - *STELLA*, *Vensim*, *Berkeley Madonna*





System Dynamics Applications

- Drug dosage
- Scuba diving - ideal gas laws
- Defibrillators - electrical circuits
- Radioactive chains
- Global warming
- Enzyme kinetics
- Cardiovascular system
- Carbohydrate metabolism
- Predator-prey and competition
- Malaria and other diseases

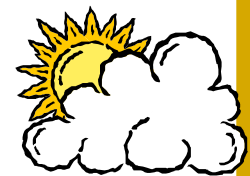




Internship: Education & Modeling



- The Shodor Foundation
 - National repository of computational science educational materials
 - www.shodor.org
 - Air pollution model on web
 - SIAM



THE SHODOR EDUCATION
FOUNDATION, INC.

<http://www.wofford.edu/ecs/>

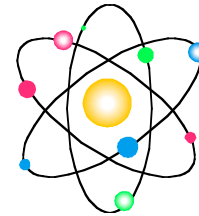


Internship: Numerical Methods

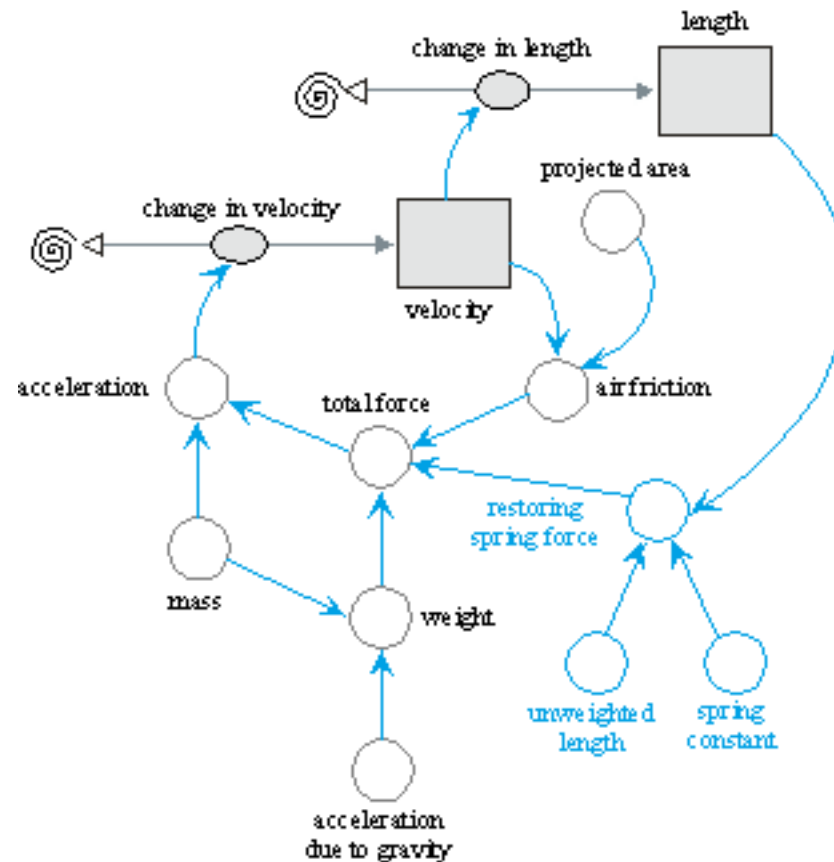
- Searched internet and found...
- Oak Ridge National Laboratory
 - 2 summers

- Now

- Graduate school in computational physics at NC A&T



Modeling Example: Motion of a bungee jumper





Internship: Modeling

- Oak Ridge National Laboratory
- Computational model of biochemical pathways
- Differential equations with only one semester of calculus and ECS



OAK RIDGE NATIONAL LABORATORY

<http://www.wofford.edu/ecs/>



Achievements

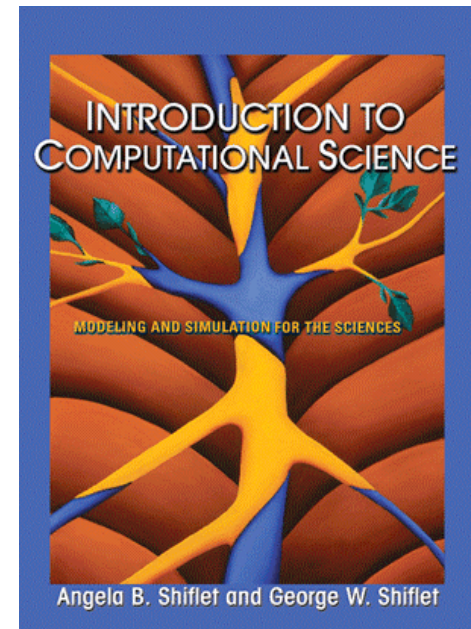
- Supercomputing Conference
- Continuation of research
- Biomedical research at ORNL
- Vanderbilt U. Medical School
 - Modeling biomechanical properties of bone





Textbook for Modeling and Simulation

- *Introduction to Computational Science: Modeling and Simulation for the Sciences*
 - Angela Shiflet and George Shiflet
 - Princeton University Press, 2006
- Files & tutorials on website in
 - *STELLA, Vensim, Madonna*
 - *Maple, Mathematica, MATLAB*
 - *Python, Excel*





Undergraduate computational science programs with internships can help fill critical need



- Computers
 - fast & cheap enough
- Networks
 - sophisticated enough
- Internet
 - pervasive and friendly enough
- Scientific visualization
 - mature enough
- Computational tools
 - Useful, yet simple, enough





The sky is not the limit



- JPL - Near Asteroid Team
- Database and computation
 - Found asteroid
- Ph.D. in Earth & Planetary Sciences
 - Rate of transfer of light through Martian atmosphere
 - Simulations
 - Numerical solutions to DEs
- Post-doc - Johns Hopkins U. Applied Physics Lab
 - Imaging spectrometer for Mars Orbiter

