Preparing the Future Workforce for Careers in Science and Engineering

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XSEDE
Extreme Science and Engineering Discovery Environment
Preparing Students

• Need for a workforce which understands both modeling and simulation principles and applications of models and data analysis at large scale
  – Requirements for high fidelity models of complex systems
  – Managing and understand large datasets – data science
Making Progress in Science

• A number of studies document the need for computational scientists
  
  – “…computer modeling and simulation are the key elements for achieving progress in engineering and science.” NSF Blue Ribbon Panel on Simulation-Based Engineering Science

  – “Unfortunately, the translation of systems biology into a broader approach is complicated by the innumeracy of many biologists” Cassman et al. Barriers to Progress in Systems Biology, Nature Vol. 438|22/29 December 2005

  – Nearly 100% of the respondents indicated that HPC tools are indispensable, stating that they would not exist as a viable business without them or that they simply could not compete effectively. IDC Study for Council on Competitiveness of Chief Technology Officers of 33 Major Industrial Firms
Crucial Tools for Manufacturing

- At Ford, HPC ...allows us to build an environment that continuously improves the product development process, speeds up time-to-market and lowers costs.
- The ongoing use of modeling and simulation resulted in new packaging and product design that propelled the brand to a leading market position over a several-year period.

Ford EcoBoost Technology

Durable coffee package for P&G
Will Pringles Fly?

High Speed Conveying Create Vortices Shedding…
…’Rocking Chips’
NOT GOOD!
Computation is Central to How Science is Done

- Computation lets us explore phenomena that are too big or complex to experiment, too small, or changes too fast or too slowly.
- Computation allows us to explore more options more quickly.
Challenges to Changing How and What We Teach

• We tend to teach in the way we were taught

• Computational science is interdisciplinary
  – Faculty workloads fixed on disciplinary responsibilities
  – Coordination across departments is superficial
  – Expertise at universities is spotty

• Major time commitments are required to negotiate new programs and develop materials

• Curriculum requirements for related fields leave little room for new electives

• Change is hard
Pathways to Reform

• Integrate computational examples into basic science and math courses
• Create general education courses that introduce simulation and modeling concepts and applications
• Combine those efforts to create formal concentrations, minors, or certificates in computational science
• XSEDE is working with institutions to assist with those activities
What Do Students Need to Know?

• Considerable discussion across many disciplines
• Difficulty working from general conceptual ideas to specific skills and knowledge
• Several efforts focused on a competency based model to arrive at consensus of the essential knowledge base
• Competencies reviewed by both academic and non-academic experts
• See
  http://hpcuniversity.org/educators/competencies/
Ohio Minor Program Example

- Undergraduate minor program
  - 6-8 courses
  - Varies based on major
- Faculty defined competencies for all students
- Reviewed by business advisory committee
- Program started in Autumn 2007
- Agreements to share students at distance, instructional modules, revenues, and teaching responsibilities

<table>
<thead>
<tr>
<th>Competencies for Undergraduate Minor</th>
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<tbody>
<tr>
<td>Simulation and Modeling</td>
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<tr>
<td>Programming and Algorithms</td>
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<td>Differential Equations and Discrete Dynamical Systems</td>
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<td>Numerical Methods</td>
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<td>Optimization</td>
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<td>Parallel Programming</td>
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<td>Scientific Visualization</td>
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<td>One discipline specific course</td>
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<td>Capstone Research/Internship Experience</td>
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<tr>
<td>Discipline Oriented Courses</td>
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Example Competencies Simulation and Modeling

• Explain the role of modeling in science and engineering
• Analyze modeling and simulation in computational science
• Create a conceptual model
• Examine various mathematical representations of functions
• Analyze issues in accuracy and precision
• Understand discrete and difference-based computer models
• Demonstrate computational programming utilizing a higher level language or modeling tool (e.g. Maple, MATLAB, Mathematica, Python, other)
• Assess computational models
• Build event-based models
• Complete a team-based, real-world model project
• Demonstrate technical communication skills
Describe the role of modeling in science and engineering

Descriptive:
Discuss the importance of modeling to science and engineering
Discuss the history and need for modeling
Discuss the cost effectiveness of modeling
Discuss the time-effect of modeling (e.g. the ability to predict the weather)
 Define the terms associated with modeling to science and engineering
List questions that would check/validate model results
Describe future trends and issues in science and engineering
Identify specific industry related examples of modeling in engineering (e.g., Battelle; P&G, material science, manufacturing, bioscience, etc.)
Discuss application across various industries (e.g., economics, health, etc.)
Flexibility in Implementation

• Adapt existing courses by adding computationally oriented modules
• Discipline oriented courses dependent on existing faculty expertise and interests
• Different subsets of required and optional competencies tied to major, required math, and example projects
Graduate Competencies

Specializations
- Discipline-Specific HPC Simulation
- HPC Application Development
- Data Intensive Computing

Core Area 2
- High Performance Scientific Computing

Core Area 1
- Intermediate Scientific Computing

Subject Areas
- Physical Sciences and Engineering
- Computer Science
- Life Sciences and Bioinformatics
Graduate Program Development

• Assumes or provides some of the background of an undergraduate

• Focus more on research skills across several disciplines
  – Dependent on expertise of current faculty

• Program at North Carolina A&T appears to do this
Computational Science Throughout the Curriculum

• Should be preparing all students to understand computation
  – “Computational thinking”
  – Building analytical skills
  – Basic understanding of modeling principles and computing skills (beyond spreadsheets)
  – Linking problem solving, mathematics, and computational methods
Progression of Activities

- Using complete models to demonstrate principles in science or mathematical concepts
- Running models to gain insights into system behavior
- Modifying models to relax assumptions
- Building new models
Examples

• Will demonstrate examples that can be used in the classroom
• Leave you with a list of resources that you can review later
• List of resources
  – https://www.osc.edu/~sgordon/workshop/materials
Question and Discussion