Overview of Computational Science and Engineering Education Programs
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Purpose of the Meeting

• Discuss pathways to integrating computational science throughout your curriculum
  – Strategies for changes in courses
  – Potential for formal concentrations
  – Identify needs for additional resources
  – Existing or adaptable instructional materials
  – Workshops for faculty
  – Other
The Need For Computational Scientists

• A number of national 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
  
  – “A persistent pattern of subcritical funding overall for SBE&S threatens U.S. leadership and continued needed advances...” International Assessment Of Research And Development In Simulation-Based Engineering And Science
  
  – 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
Examples of Modeling Problems

• Tracing the spread and evolution of disease ([http://supramap.osu.edu/](http://supramap.osu.edu/))
• Collaborations to explore historical and contemporary events and social interaction ([http://www.ichass.illinois.edu/Projects/Projects.html](http://www.ichass.illinois.edu/Projects/Projects.html))
• Predicting the impacts of earthquakes ([http://nees.org/](http://nees.org/))
• Designing and testing new nanomaterials and devices ([http://nanohub.org/](http://nanohub.org/))
• Discovering oil reserves ([http://access.ncsa.illinois.edu/Stories/oil/](http://access.ncsa.illinois.edu/Stories/oil/))
XSEDE Education Program Goals

• Prepare the current and next generation of researchers, educators and practitioners.
• Create a significantly larger and more diverse workforce in STEM.
• Inculcate the use of digital services as part of their routine practice for advancing scientific discovery.
XSEDE Education Program Services

• Campus Visits
• Assistance with program creation
• Workshops for faculty and students
• Repository of shared materials
• Other resources
Promoting Formal Academic Programs

• XSEDE Education program is focused on assisting with the initiation and enhancement of formal computational science and engineering programs
  – Both undergraduate and graduate programs
  – Most sustainable way to help achieve the long-term project goals by producing a savvy workforce
  – Reduce the barriers to program adoption by
    • Providing program models
    • Solidifying a virtual community to share experiences
    • Providing faculty professional development
Creating Computational Science Programs

• Inherently interdisciplinary
  – Science, engineering, or social science domain
  – Mathematics
  – Computer science

• Expertise often dispersed across multiple departments

• Difficulty of negotiating requirements and responsibilities
Benefits to Students

• Prepare them for a variety of new careers
• Use of modeling as inquiry-based learning
  – Students are actively engaged in the learning process
  – Students gain deeper insights and have higher retention rates for the information
  – Facilitates the integration of information across academic disciplines – math, science, engineering, computer science
Model Community College Program

• Associate of Science degree with concentration in computational science
• Created competencies for science majors in two-year schools along with a concentration in computational science
  – http://www.rrscs.org/associate
  – Program at Stark State College in Ohio
    • http://www.starkstate.edu/academic-programs/computational-science
The Curriculum

• Associate of Science with all of the related requirements

• Five new courses were to be designed for this new program:
  – Computational Science Methods
  – Modeling and Simulation
  – Introduction to Computational Biology
  – Introduction to Computational Chemistry
  – Introduction to Computational Physics
Competencies in Computational Biology

- Explain the role of computational science in biology
- Demonstrate the use of database search engines and information retrieval methods
- Demonstrate sequence analyses
- Demonstrate basic phylogenetic tree construction, manipulation and analysis
- Discuss basic protein structure and function
- Discuss the fields of proteomics and genomics
- Introduce field of computational biomodeling
- Full list at: http://www.rrscs.org/sites/rrscs.epn.osc.edu/files/docs/computationalbiology.pdf
Other Competencies

- Modeling and Simulation
  - [http://www.rrscs.org/sites/rrscs.epn.osc.edu/files/docs/simandmodeling.pdf](http://www.rrscs.org/sites/rrscs.epn.osc.edu/files/docs/simandmodeling.pdf)

- Computational Science Methods
Choices for Implementation

• Adapt existing courses by adding computationally oriented modules
• Discuss the creation of a formal program and its requirements
• Take advantage of XSEDE and other models
  – Professional development for faculty
  – Shared educational modules
  – Access to computational resources beyond the desktop
Developing Faculty Expertise

• Faculty professional development workshops
  – Two to six day workshops on a variety of topics
    • Computational thinking
    • Computational science education in science and engineering domains
  – Focus on local/regional audiences to reduce travel costs
  – Subsidies for faculty to travel to workshops at other sites
Repository of Shared Materials

- Developing a repository of computational science education materials
  - Reviewed by professional staff and faculty
  - Indexed by subject and a detailed competency-based ontology
  - Goal: trusted, comprehensive source of information for computational science educators
  - [http://hpcuniversity.org/resources/search/](http://hpcuniversity.org/resources/search/)
XSEDE and Other Resources

• Online learning modules
  – www.xsede.org/training1

• Science Gateways
  – https://www.xsede.org/gateways-listing

• Special workbench tools
  – Biology workbench http://www.ngbw.org/
Some Other Opportunities

• Journal of Computational Science Education
  – www.jocse.org
  – Peer reviewed article on computational science education experiences

• Become a reviewer or contributor to the online repository
Questions and Discussion
Providing a Curriculum Model

• Based on our experience in Ohio creating an interdisciplinary, inter-institutional minor program in computational science
• Effort supported by an NSF grant
• Allowed us to work through many of the issues associated with creating an interdisciplinary program
• Demonstrated the feasibility of an interdisciplinary, inter-institutional program
• See http://hpcuniversity.org/educators/competencies/
Program Requirements

• Created a competency-based curriculum
  – Provides detailed outlines of the background and skills desired for students completing the program
  – Bridged the differences across disciplines
  – Allows for flexibility in implementation to fit the program into multiple institutional situations and majors with different backgrounds and focus areas

• Serves wide range of needs
  – Provides essential skills for all students regardless of whether they complete the minor
Undergraduate minor program overview

- Undergraduate minor program
  - 4-6 courses
  - For majors in variety of fields
- Faculty defined competencies for all students
- Reviewed by business advisory committee
- Currently being updated to reflect changes in hardware and software technologies
- Requirements adjusted to reflect the needs of different majors

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<tr>
<th>Competencies for Undergraduate Minor</th>
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<tr>
<td>Simulation and Modeling</td>
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<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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