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Overview of Computational Science and Engineering Education Programs

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XSEDE

Extreme Science and Engineering Discovery Environment

NSF

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/
- Collaborations to explore historical and contemporary events and social interaction (http://www.ichass.illinois.edu/Projects/Projects.html)
- Predicting the impacts of earthquakes (http://nees.org/)
- Designing and testing new nanomaterials and devices (http://nanohub.org/)
- Discovering oil reserves (http://access.ncsa.illinois.edu/Stories/oil/)
- Designing new packaging (http://phx.corporate-ir.net/phoenix.zhtml?c=104574&p=irol-newsArticle&ID=651774&highlight)
- Discovering how the brain works (http://www.compete.org/publications/detail/503/breakthroughs-in-brain-research-with-high-performance-computing/)

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.

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, colleges, institutions
- Difficulty of negotiating requirements, responsibilities, and institutional arrangements

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

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

Competencies for Undergraduate Minor
Simulation and Modeling
Programming and Algorithms
Differential Equations and Discrete Dynamical Systems
Numerical Methods
Optimization
Parallel Programming
Scientific Visualization
One discipline specific course
Capstone Research/Internship Experience

Undergraduate Compentencies

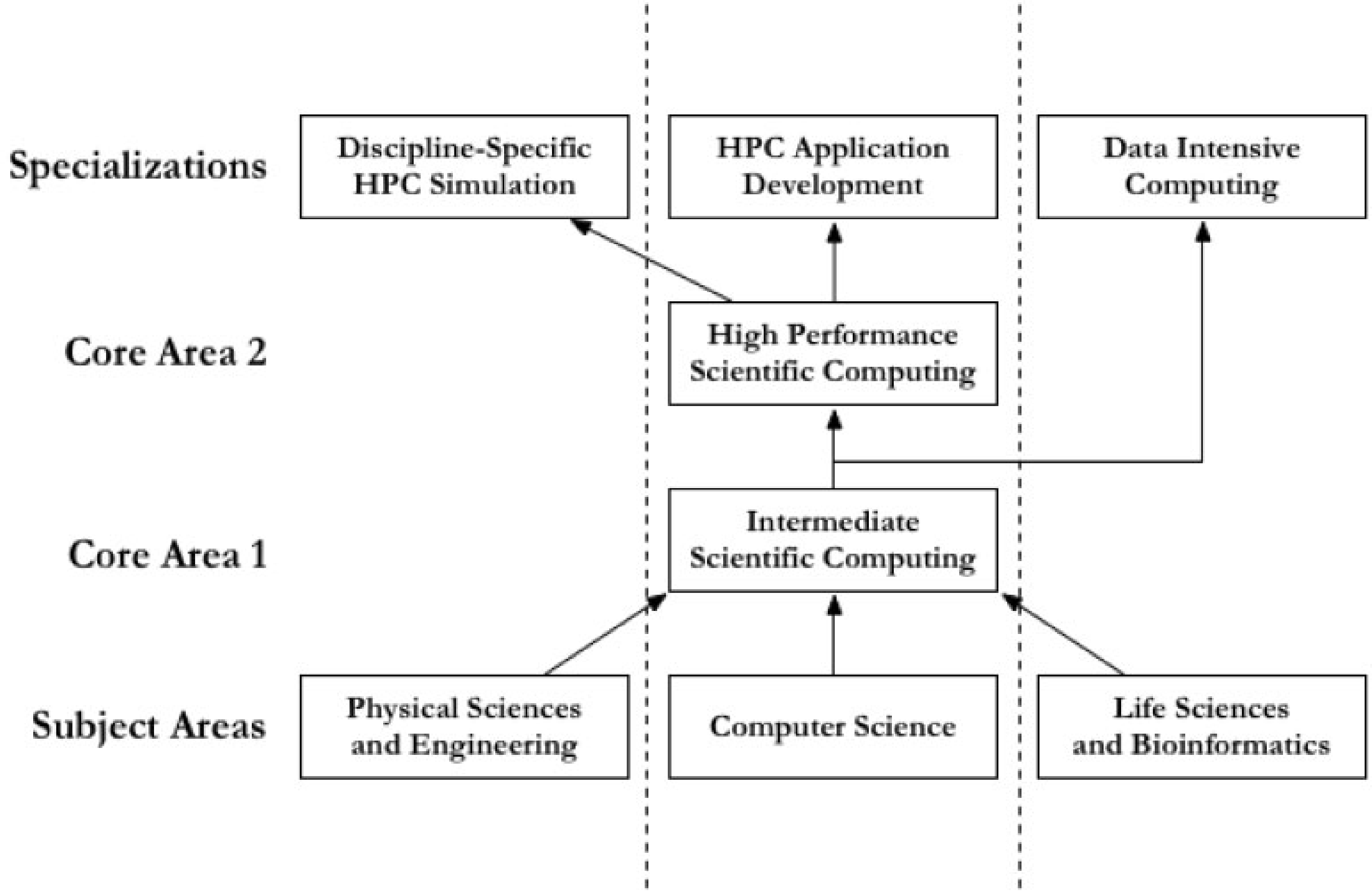
- Model competencies for undergraduate program in Ohio
  - http://www.rrscs.org/sites/rrscs.epn.osc.edu/files/competency_2012.pdf

Flexibility in Implementation

- Adapt existing courses by adding computationally oriented modules or focus on new target audience
- 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 Level Competencies

- Assumes some of the background of an undergraduate
- Focus more on research skills
- Core areas focus on the computer science and related modeling skills
- Need to branch into a wider array of specializations based on the nature of the graduate program


Specializations
Core Area 2
Core Area 1
Subject Areas
Discipline-Specific HPC Simulation
HPC Application Development
Data Intensive Computing
High Performance Scientific Computing
Intermediate Scientific Computing
Physical Sciences and Engineering
Computer Science
Life Sciences and Bioinformatics

Intermediate Level Scientific Computing

Intermediate Level Scientific Computing Major Competencies
Ability to contribute code in the programming language of greatest importance in the research domain, either Fortran or C
Students will be introduced to basic debugging techniques
Understand number representation
Understand numerical errors
Students will be introduced to software engineering best practices
Ability to identify efficient file formats
Create a program that uses at least one widely used numerical library
Students will be introduced to the concepts of algorithm complexity
Students will be introduced to serial program optimization concepts and techniques
Students will understand verification and validation principles
Students will be introduced to Monte Carlo methods

Introduction to HPC

Intro To High Performance Scientific Computing Major Competencies
Students will be introduced to parallel architectures and execution models
Students will be introduced to memory models for parallel programming
Students will understand the principles of how to match algorithms, applications, and architectures
Students will understand the concept of application scalability
Students will understand code performance metrics
Students will be introduced to parallel programming methods and concepts
Data Intensive Computing
Data management
Understanding fault tolerance
Students will understand basic scientific visualization concepts

Domain Specific Competencies

- Still need to be developed in detail
- Tied to the expertise at each campus that institutes a program
- Broad categories
  - Advanced HPC
  - Advanced Data Management
  - Major modeling efforts in each field of science and engineering

Draft Competencies for Graduate Program

- Core graduate competencies
  - http://www.rrscs.org/sites/rrscs.epn.osc.edu/files/graduate_competencies_v6.pdf

XSEDE Assistance

- XSEDE can provide help to
  - Facilitate discussions among faculty and administrators on campus
  - Visit campuses and help work through program organization
  - Provide access to example program agreements and instructional materials
  - Provide faculty professional development

Discussion Questions

- Address these questions:
  - What are the areas of science and engineering where your institution has computational science expertise that could be integrated with undergraduate and graduate programs in computational science?
  - What is the potential for an inter-institutional program?
  - What are the next steps in creating such a program?