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A New Graduate Minor Program in Computational Science

www.csci.psu.edu

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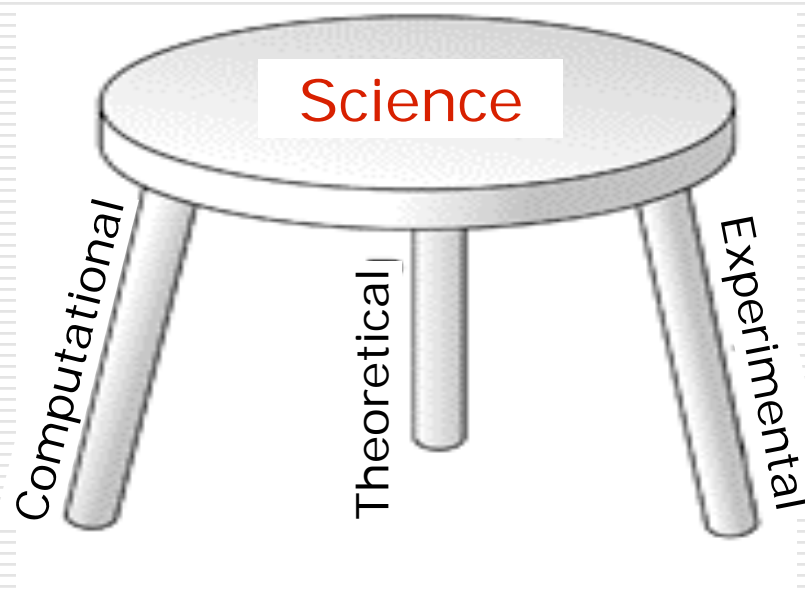
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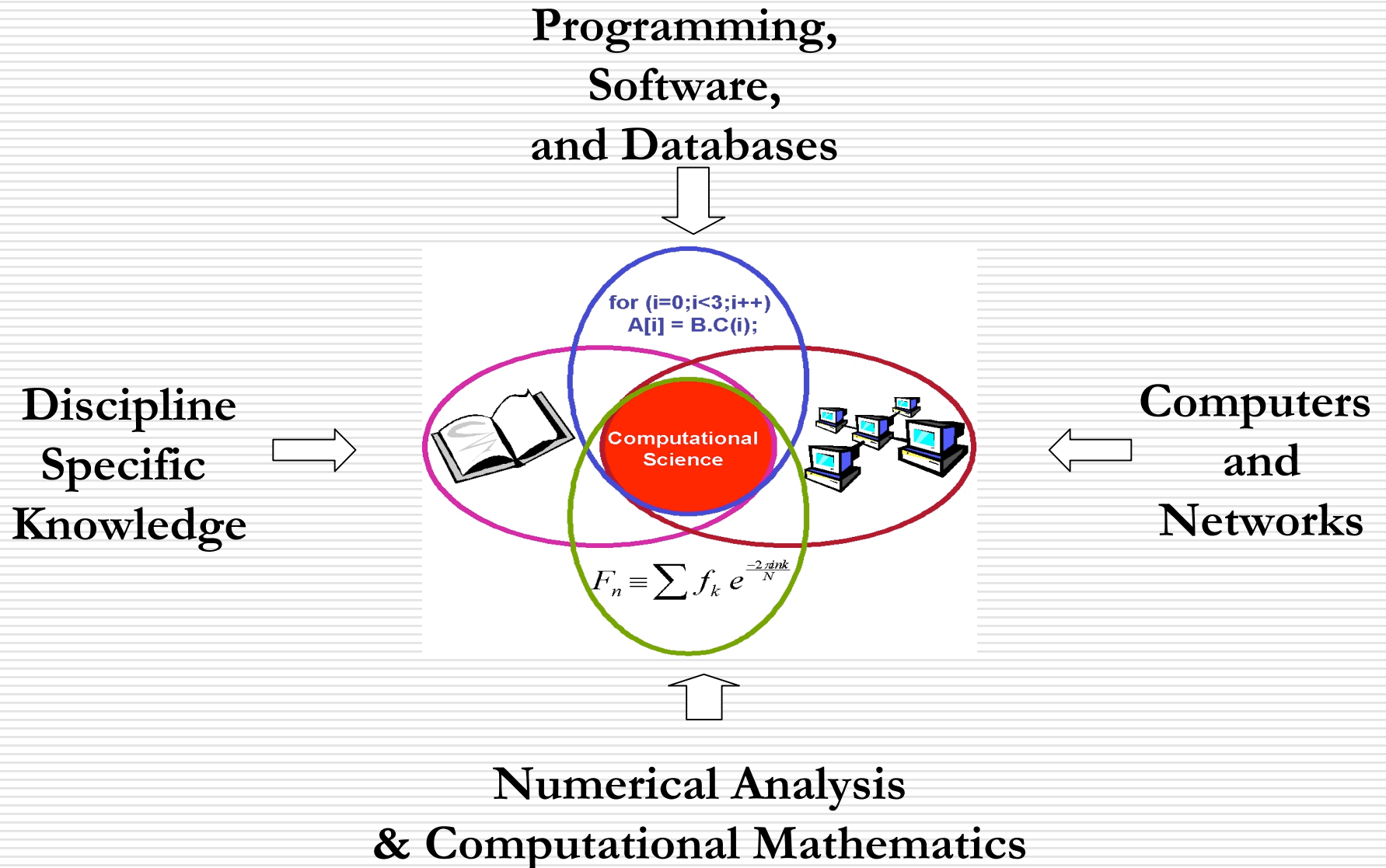
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What is Computational Science?

- **IEEE:**
“... science (and engineering) that is "computational" as opposed to "experimental" or "theoretical”
- **Krell Institute:**
“... computational science involves using computers to study scientific problems and complements the areas of theory and experimentation in traditional scientific investigation.”
- **SIAM:**
“Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics and computer science. CSE focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems. We believe that CSE will play an important if not dominating role for the future of the scientific discovery process and engineering design.”



What is Computational Science?



A New Graduate Minor in Computational Science

Core Requirements:

- Computational Science Tools (2 cr.)
- Computational Science Invited Lectures (1 cr.)
- And two of these (3 cr. each):
 - AERSP 424: Advanced Computer Programming
 - CSE 557: Concurrent Matrix Computation *OR*
NucE 530: Parallel and Vector Computing
 - Math 523: Numerical Analysis
- M.S. degree Minor (9 credits)
 - Core Requirements (9 cr.)
- Ph.D. degree Minor (15 credits):
 - Core Requirements (9 cr.)
 - And two courses from the list of 73 CSci courses from 20 different departments (6 cr.)
- The courses can also be applied towards their major degree
- Previously, called the Graduate Minor in High Performance Computing

Advanced Computer Programming

AERSP 424 (Fall semesters)

This course presents an advanced view of computer programming, mainly using Java and C++. The use of current operating systems (e.g. Linux and Unix) and compilers (e.g. gcc) will also be presented. Object Oriented Programming will also be discussed in detail. Object Oriented Programming is quite different than functional or procedural programming, and it is difficult to learn on your own. The differences and similarities between Java and C++ will also be discussed. Hands-on programming will be a key part of the course. As Robert Glass says in his "Facts and Fallacies" book, it will be important for you to be able to read codes (as well as write them).

The goal of this course is to introduce and study key concepts related to computer programming for scientific and engineering applications.

Prerequisite: CMPSC 201C; and MATH 220; MATH 250 or MATH 251

www.personal.psu.edu/lnl/424pub

(also Software Engineering, AERSP 440, is offered each Spring)

Parallel Computing

(CSE 557 or NucE 530)

- They can take one of these as a Core course:
 - CSE 557 CONCURRENT MATRIX COMPUTATION (3)
 - This course discusses matrix computations on architectures that exploit concurrency. It will draw upon recent research in the field. Prerequisite: CSE 451 , CSE 455 , CSE 457 , MATH 451 , or MATH 455
 - NUCE 530 PARALLEL/VECTOR ALGORITHMS FOR SCIENTIFIC APPLICATIONS (3)
 - Development/analysis of parallel/vector algorithms (finite-differencing of PDEs and Monte Carlo methods) for engineering/scientific applications for shared and distributed memory architectures. Prerequisite: AERSP 424 or CSE 457

Numerical Analysis

Math 523

- Matrix computation and linear system
- Nonlinear equations and optimization
- Data and signal analysis
- Numerical Quadrature
- Monte Carlo integration
- Differential equations

Seminars (Required)

AERSP 590

Computational Science Tools, Fall Semesters, 2 credits

- High Performance Computing Systems
- Networking and Collaboration
- Numerical libraries.
- Programming and Software
- Profiling / debugging / code optimization.
- Statistics and Probability
- Graphics and Visualization

• Computational Science Invited Lectures, Spring Semester, 1 cr.

- This course presents the research of fourteen prominent computational science researchers. Each speaker discusses the latest research in their technical areas. Speakers from areas such as engineering, physics, chemistry, software engineering, materials science, intelligent systems, computer science, statistics, and mathematics.

- <http://www.csci.psu.edu/seminars.html>

List of Other 70 Courses

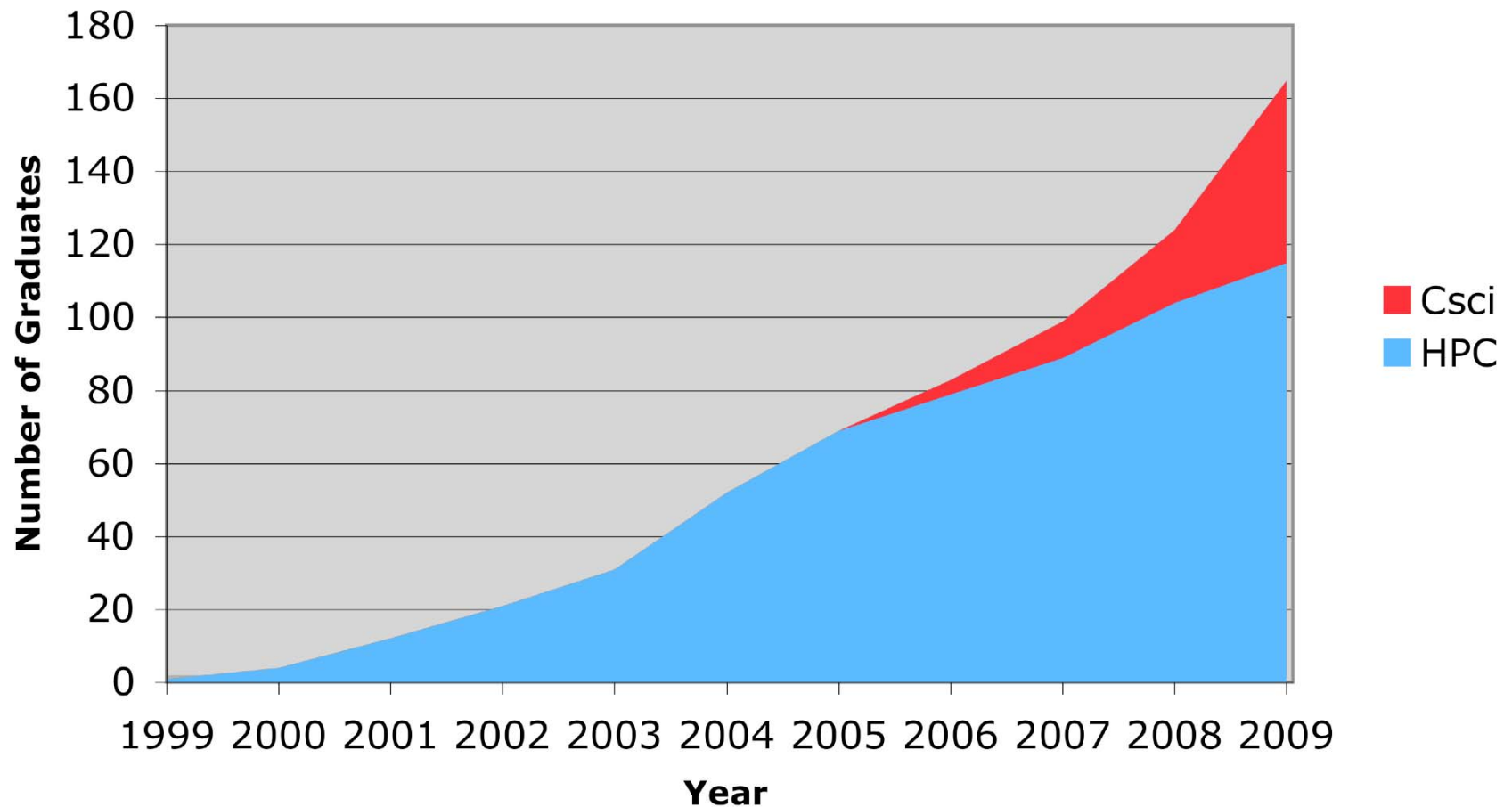
- Agricultural Engineering:
 - Boundary element analysis
- Acoustics:
 - Computational acoustics
- Aerospace Engineering:
 - Intro. to Computational Fluid Dynamics
 - Stability of Laminar Flows
 - Turbulence and Appl. to CFD: RANS
 - Adv. anal. and comp. of turbomachinery
 - Finite Element Methods
- Architecture:
 - Topics in Visualization
- Civil Engineering
 - Structural Analysis
 - Evolutionary Algorithms
- Chemical Engineering:
 - Numerical methods in chemical engineering
 - Optimization in Biological Systems
- Chemistry:
 - Quantum mechanical elect. structure
 - Computer Simulations for Physical Scientists
- Computer Science:
 - Computer Graphics
 - Operating Systems Design
 - Computer Networks
 - Computer architecture
 - Parallel processors and processing
 - Multiprocessor architecture
 - Interconnection networks in parallel computers
 - Numerical Linear Algebra
 - Advanced Topics in Scientific Computing
- Electrical Engineering:
 - Introduction to Neural Networks
 - Numerical methods in electromagnetics
 - Graphs, Algorithms, and Neural Networks
 - Intelligent Control
- EGEE
 - Numerical Modelling
- Engineering Science:
 - Simulation and design of nanostructures
 - Brain Computer Interfaces
 - Finite element methods
 - Nonlinear finite element methods
- GeoScience
 - Mathematical Modeling in the Geosciences
 - Computational Geomechanics
- Industrial Engineering:
 - Distributed Systems and Control
 - Using simulation models for design
- Information Science:
 - Advanced Topics in Databases
 - Simulating Human Behavior
- Mathematics:
 - Numerical linear algebra
 - Num. solution of ord. differential eqtns.
 - Num. solution of partial differential eqtns.
 - Numerical optimization techniques
 - Finite element methods
 - Applied Math I
 - Intro to Multigrid and Domain Decomposition
- Materials Science:
 - Computational Thermodynamics
 - Computational Materials Science II:
 - Polymeric Materials: Computation
- Mechanical Engineering:
 - Comp. heat trans. and fluid mechanics
 - Turbulence & Appl. to CFD: DNS and LES
 - Computational methods for shear layers
 - Computational methods in transonic flow
 - Comp. methods for recirculating flows
 - Grid Generation
- Meteorology:
 - Numerical weather prediction
 - Advances in numerical weather prediction
- Nuclear Engineering:
 - Neutron Transport Theory
 - Introduction to Monte Carlo Methods
- Physics:
 - Computational physics
 - Computational physics II
 - Computer Simulation of Materials
- Petroleum:
 - Numerical Solution Flow in Porous Media
 - Numerical Reservoir Simulation
- Statistics:
 - Statistical Computing
 - Applied Statistics
 - Stochastic Processes and Simulation
 - Statistical Computing
 - Stochastic Dynamics of the Living Cell
 - Data Mining

The Students

- 80 Currently Enrolled
- 124 have graduated:
 - 20 Computational Science Minors awarded (2006-Present)
 - 104 High Performance Computing Minors awarded (1999-2008)
- Complete list of students at:
 - <http://www.csci.psu.edu/stulist.html>

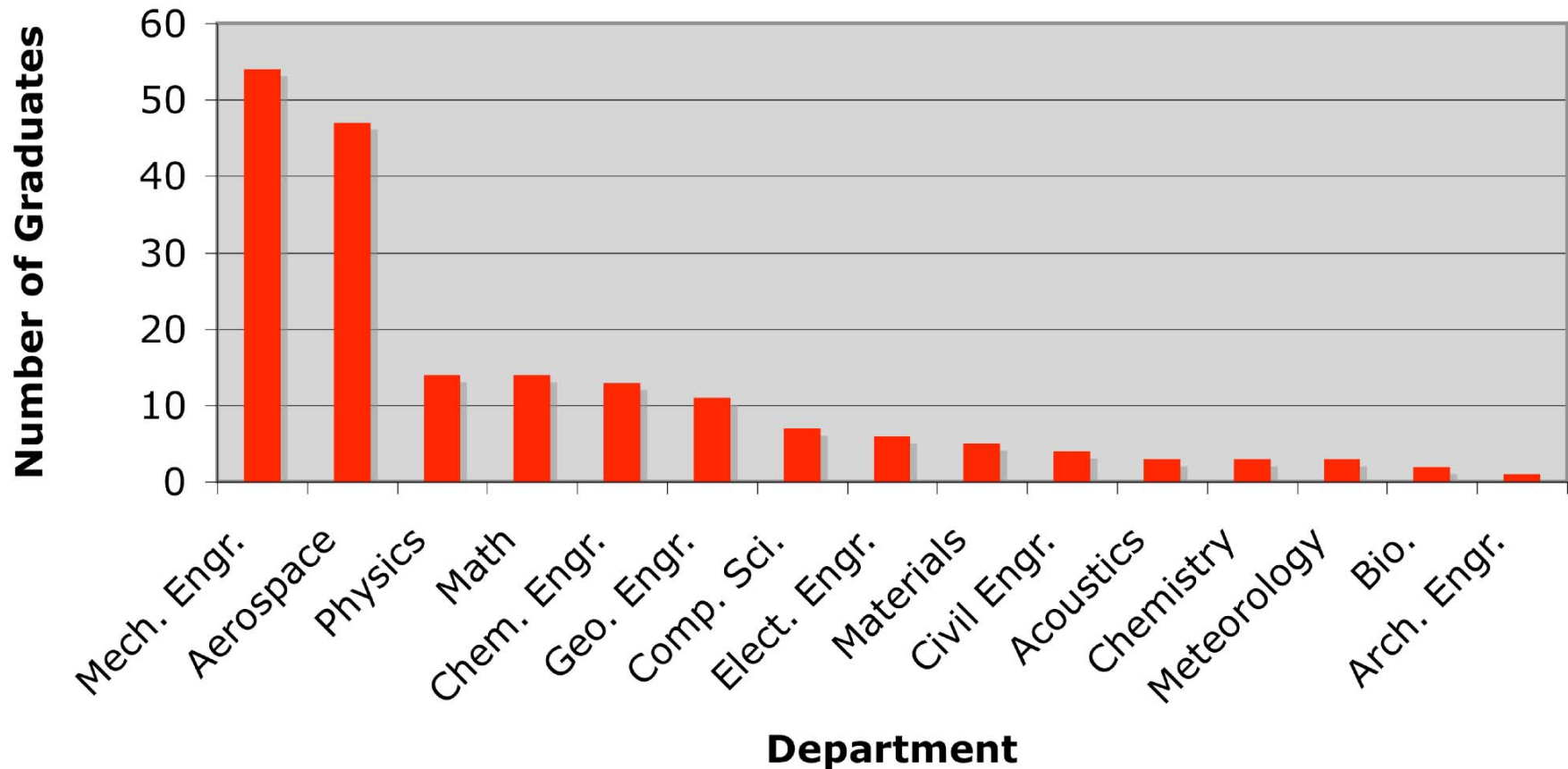
Students

Cummulative Number of Grad Minor Degrees Awarded (www.csci.psu.edu)



Students

Number of Grad Minors by Department



Conclusions

- Computational science will continue to be more and more important
- A Grad Minor in CSci is a good approach, the students get credit for learning material beyond their major discipline
- We have considered creating a Ph.D. program in Computational Science also...

Questions ?

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