
A Plan for a Computational Science Program at UTK

Background

- Many of the outstanding research problems in science and engineering today are computationally challenging, requiring a new scientific approach
- As one report points out,

“The use of modern computers in scientific and engineering research and development over the last three decades has led to the inescapable conclusion that a third branch of scientific methodology has been created. It is now widely acknowledged that, along with traditional experimental and theoretical methodologies, advanced work in all areas of science and technology has come to rely critically on the computational approach.”

- This methodology represents a new intellectual paradigm for scientific exploration, one which opens up a wide range of new opportunities to solve problems that were previously inaccessible.



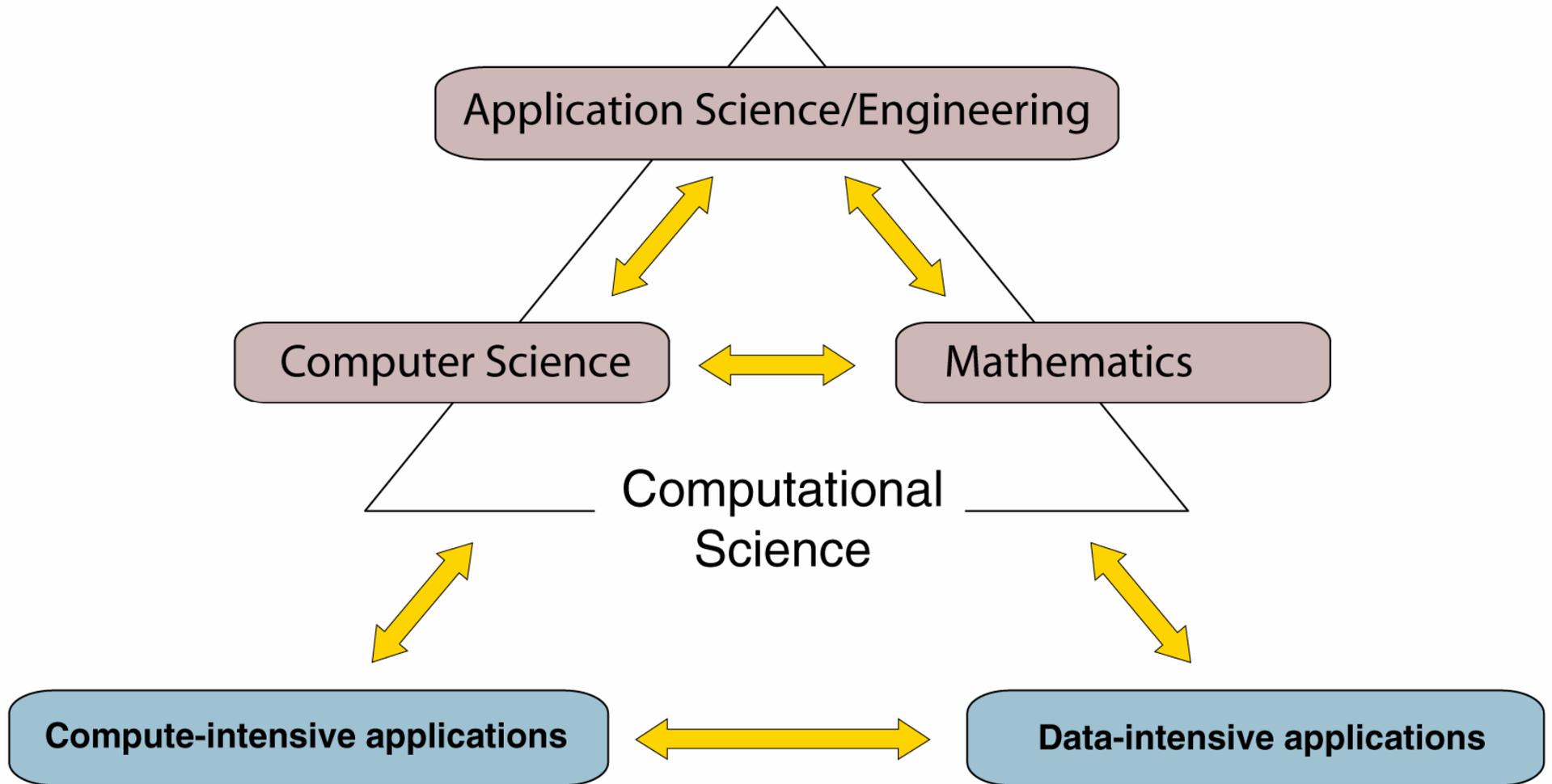
Computational Science Defined

Computational science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems.

Computational science fuses three distinct elements:

- *algorithms* (numerical and non-numerical) and *modeling and simulation software* developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems,
- *computer and information science* that develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems; and
- *the computing infrastructure* that supports both the science and engineering problem solving and the developmental computer and information science.

Relationships between Computational Science, Computer Science, Mathematics and Applications



Substantial Growth Multidisciplinary R&E Initiatives at UTK/ORNL

- Innovative Computing Laboratory
- The Institute for Environmental Modeling
- UT-ORNL Graduate School of Genome Science & Technology
- Joint Institute of Computational Sciences
- Joint Institute of Biological Sciences
- Joint Institute for Neutron Sciences
- as well as others.

Computational Science As An Emerging Academic Pursuit

- Many Programs in Computational Science
 - College for Computing
 - Georgia Tech; NJIT; CMU; ...
 - Degrees
 - Rice; Utah; UCSB; ...
 - Minor
 - Penn State; U of Arizona; Indiana U; ...
 - Certificate
 - Old Dominion; U of Georgia; Boston U; ...
 - Concentration
 - Cornell; Northeastern; Colorado State; ...
 - Courses

Some Existing Graduate Programs in Computational Science

(http://www.siam.org/students/resources/cse_programs.php)

Clemson University	Computational Science & Engineering Program (CS&E) Master's Degree in CS&E	Seoul National University	Computational Science and Technology	University of Iowa	Applied Mathematics and Computational Sciences Program PhD in Interdisciplinary AMCS Program
ETH, Zurich, Switzerland	Rechnergestützte Wissenschaften (CSE)	Stanford University	Institute for Computational and Mathematical Engineering (ICME)	University of Manchester	Applied Numerical Computing
George Mason University	Computational Sciences and Informatics	State University of New York Brockport	Computational Sciences This is an interdisciplinary independent degree - granting program, with participation of several departments. Both undergraduate and graduate degrees offered. Program has core faculty plus members from other departments. The program offers access to several parallel supercomputers.	University of Manchester	MSc in Computational Science
George Washington University Virginia Campus	Computational Sciences	State University of New York Stony Brook (SUNY/SB)	Computational Applied Mathematics Program.	University of Maryland, College Park	Applied Mathematics and Scientific Computation Program (AMSC) Interdisciplinary MA and PhD programs, with concentrations in Applied Mathematics and in Scientific Computation. Certificate in Scientific Computation also available.
Georgia State University	M.S. in Scientific Computation	Syracuse University	Computational Science Program (CPS) MS and PhD in Participating Dept with Certificate in Program	University of Michigan	Doctoral Program in Scientific Computing Certificate in scientific computing appended to departmental degrees
Helsinki University of Technology	Computational Science and Engineering MSc program for most fields of Engineering	Technische Fachhochschule Berlin, University of Applied Sciences	Computational Engineering Master's degree in Computational Engineering	University of Minnesota	Scientific Computation Program MS and Ph.D degrees in Scientific Computation
Indian Institute of Science	Computational Science and Engineering	Technische Universität München	International Masters Program in CSE	University of Oxford	MSc degree in Mathematical Modelling and Numerical Analysis; D. Phil. degree in Numerical Analysis.
Indiana University at Bloomington	Scientific Computing Program Graduate Level Minor	Technischen Universität Braunschweig	Computational Sciences in Engineering Master's degree in CSE. PhD in participating departments.	University of Southern Mississippi	Scientific Computing
KTH, Stockholm, Sweden	International Programme in Scientific Computing MS program	Universität Erlangen-Nürnberg	Computational Engineering Bachelor's and Master's degrees	University of Texas, Austin	Texas Institute for Computational and Applied Mathematics (TICAM) Program MS and PhD in computational and applied mathematics
Mississippi State University	Computational Engineering	University of California, Santa Barbara	Computational Science and Engineering	University of Utah	Computational Engineering & Science Graduate Program (CE&S)
National Singapore University	Computational Science	University of Colorado, Denver	PhD Degree in Applied Mathematics with a Computational Mathematics Option	Uppsala University	Department of Scientific Computing
New York University (NYU)	Masters Degree Program in Scientific Computing.	University of Delaware	Graduate Program in Scientific Computation.	William and Mary	Graduate Studies in Computational Science. Studies in computational science cluster leading to certificate
Ohio University	M.S. in Mathematics - Computational Track	University of Houston	Computational Sciences Initiative Interdisciplinary graduate certificate program		
Old Dominion University	Certificate in Computational Science & Engineering	University of Illinois, Chicago	Computational Science and Applied Mathematics program. PhD in Mathematics with Major in Computational Science cluster of Mathematical Computer Science program or any cluster in Applied Math program	Carnegie Mellon University	MS in Computational Finance
Oxford University Computing Laboratory	Graduate Courses in Computing.	University of Illinois, Urbana	Computational Science and Engineering (CSE) option MS and PhD in Participating Depts with Minor Certificate in CS&E	Cornell University	Financial Engineering Option.
Pennsylvania State University	High Performance Computing HPC Graduate Minors in High Performance Computing, at the M.S. and Ph.D. levels.	University of Iowa	Applied Mathematics and Computational Sciences Program PhD in Interdisciplinary AMCS Program	Columbia University	Masters Program in Financial Engineering
Princeton University	Program in Applied and Computational Mathematics			Purdue University	Computational Finance Program
Purdue University	Computational Science and Engineering. MS and PhD programs.			University of Chicago	Master of Science in Financial Mathematics
Rensselaer Polytechnic Institute	Computational Science and Engineering Program. Graduate certificate program			University of Michigan	MS in Financial Engineering
Rice University	Computational Science & Engineering (CS&E) Proposed MS and PhD in CS&E			University of Toronto	Mathematical Finance
San Diego State University	Computational Science				

Computational Finance

Objectives of This Effort

- To support interdisciplinary programs in the sciences.
- To train and educate students and young investigators, as well as established researchers, in the effective use of techniques and equipment for advanced parallel computational systems.
- To foster the exchange of knowledge and experiences between universities, government laboratories and industry.
- To attract students into science and technology career paths and to encourage educators to use high performance computing for teaching and demonstrating scientific and mathematical principles.
- To encourage the advancement of computationally intensive science by promoting the use of high-performance computers, visualization, and other parallel computational tools.
- To provide a forum for the evolution of Computational Science as a basic part of curriculum in many fields.
- To work as partners with the computer industry for achieving major advances in computer technology.

Possibilities Paths

- Concentration in Computational Science
 - Original plan

- Minor in Computational Science
 - Modeled on: Intercollegiate Graduate Statistics Program

Possible Model: Intercollegiate Graduate

Statistics Program <http://bus.utk.edu/stat/igsp/courses.htm>

- Masters and PhD students in a discipline can get either a *Minor* in Stat along with their degree;
- This model is a formal UT Program, well understood by the University and viewed as a success
 - Suggested as possible model by Dean Mayhew
 - Established in 1988 (lots of experience to draw on)
 - Provides a detailed model we can follow or modify
- On student's transcript: PhD or MA/MS in X with "... Minor in Computational Science" (or something similar)
- Key difference: Our *Intercollegiate Graduate Program in Computational Science (IGPCS)* currently has no underlying Department/School of Computational Science

Possible IGPCS Curriculum

- Courses divided into level A and level B:
 - Level A: Introductory or graduate-level applied courses in Computational Science (CaS).
 - Possible examples: **Intro to Scientific Computing** (3 hours); **Advanced Scientific Computing** (3 hours)
 - Current Stat program has 10 level A courses, drawn from both Statistics Dept. and other departments in the program
 - Level B: Graduate-level applied courses in CaS with Level A (or equivalent) prerequisites
 - Possible examples: **Scientific Visualization** (3 hours); **Mathematical Modeling** (3 hours), approved elective courses in departmental plan, **possibly a seminar approved by committee; internship at ORNL**
 - Current Stat program has 20 level B courses, also from various program departments
 - Courses added to level A and B by approval of the IGPCS Executive Committee (Must meet all normal University requirements as well)
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How It Might Work For Students

Degree Program	Recognition Sought	Requirements
Master's in Home Dept.	Minor in Computational Science	9 hrs.: 6 @ level A, 3 @ level B
Doctorate in Home Dept.	Science	15 hrs.: 6 @ level A, 9 @ level B

- Open to all students in departments with approved minor
- Home departments establish an approved program/list of courses for their students, which is approved by executive committee. Students choose courses from appropriate list
- Level A courses must be approved sequence
- Home dept. must verify fulfillment of non-CalS degree requirements
- ORNL internship strongly encouraged

Steps to Implement this Model

- Initial IGPCS Executive Committee is formed
- Participating departments put forward the courses/descriptions for the Level A & B courses
- Executive committee works with other IGPCS faculty to evaluate courses and identify relevant sequences among them
- Departments propose a program (course options, suitably sequenced) for their students
- Executive Committee reviews and either accepts or returns for modification

Program Administration

- IGPCS Executive Committee
 - Subset of the Program Faculty
 - 1 representative from each of the colleges involved, appointed by the Dean of that college
 - Renewable 2 year terms
 - Responsible for setting program requirements, approving courses and department programs, etc.
 - Executive Committee Chair could be the JICS Director
 - Role of JICS?
- IGPCS Program Faculty
 - Any faculty member, assistant professor or above in rank, nominated by department head and approved by executive committee
 - Responsible for teaching program courses, directing student research, serving on student committees

Departments Who Have Identified a Track Within Their Department

- Animal Science
 - Graduate Concentration in Computational Science
- Chemical Engineering
 - Graduate Concentration in Molecular-Level Simulation
- Computer Science
 - Graduate Concentration in Computational Science
- Engineering Science
 - Graduate Certificate in Computational Fluid Dynamics
- Geography
 - Graduate Concentration in Computational Science
- Mathematics
 - Graduate Concentration in Computational Science
- Physics
 - Graduate Concentration in Computational Science
- School of Information Sciences
 - Graduate Concentration in Computational Science:
 - Human Computer Interaction
 - Knowledge Mining

Roadmap

■ December 2005 – February 2006

- ❑ Group meets and agrees on some initial version of the plan
- ❑ Group members take the initial draft back to departments; iterate on the plan via e-mail January – early February 2006
- ❑ Updated version of the plan is presented to the Chancellor, Dean's meeting, and/or the Graduate Council
- ❑ Group meets to finalize the plan
- ❑ Overall program plan is presented in a letter to Chancellor/Chancellor's staff for approval. That approval would transform our working group, or some subset of it into the initial Executive Committee for the new Computational Science Program.

■ March – April 2006

- ❑ Catalogue copy for new courses is developed by each department that wants to offer Computational Science Minor
- ❑ Departmental program plans are reviewed and approved by the Computational Science Executive Committee as meeting program requirements
- ❑ Catalogue copy is submitted to each department. At this point, the catalogue copy would begin the normal process up the hierarchy in order to be approved and included in the catalogue for 07-08.

How This Could Work

- Each department would define what it means by a concentration in computational science.
 - This would be done in the form of a track in relevant courses.
 - This could include interdisciplinary courses.
- Director of the Joint Institute for Computational Science (JICS) would have oversight on the efforts and help coordinate the efforts with a representative from each participating department.
- Each program would be strongly encouraged to require ORNL internship.
- The degree itself will be awarded within the department that the student is enrolled.