A Plan for a Computational Science Program at UTK
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

**Clemson University**  
**Program:** Computational Science & Engineering Program (CSE)  
**Degree:** Master's Degree in CSE

**ETH, Zurich, Switzerland**  
**Program:** Rechnen und Wissenschaftliches Rechnen (CSE)

**George Mason University**  
**Program:** Computational Sciences and Informatics

**George Washington University Virginia Campus**  
**Program:** Computational Sciences

**Georgia State University**  
**Program:** M.S. in Scientific Computation

**Helsinki University of Technology**  
**Program:** Computational Science and Engineering  
**Degree:** MSc program for most fields of Engineering

**Indian Institute of Science**  
**Program:** Computational Science and Engineering

**Indiana University at Bloomington**  
**Program:** Scientific Computing Program  
**Minor:** Graduate Level Minor

**KTH, Stockholm, Sweden**  
**Program:** International Programme in Scientific Computing MS program

**Mississippi State University**  
**Program:** Computational Engineering

**National Singapore University**  
**Program:** Computational Science

**New York University (NYU)**  
**Program:** Masters Degree Program in Scientific Computing

**Ohio University**  
**Program:** M.S. in Mathematics - Computational Track

**Old Dominion University**  
**Program:** Certificate in Computational Science & Engineering

**Oxford University Computing Laboratory**  
**Program:** Graduate Courses in Computing

**Pennsylvania State University**  
**Program:** High Performance Computing  
**Tracks:** HPC Graduate Minor in High Performance Computing, at the M.S. and Ph.D. levels.

**Princeton University**  
**Program:** Program in Applied and Computational Mathematics

**Purdue University**  
**Program:** Computational Science and Engineering  
**Degrees:** MS and PhD programs

**Rensselaer Polytechnic Institute**  
**Program:** Computational Science and Engineering Program  
**Certificate:** Graduate certificate program

**Rice University**  
**Program:** Computational Science & Engineering (CSE)  
**Degrees:** MS and PhD in CSE

**San Diego State University**  
**Program:** Computational Science

**Social National University**  
**Program:** Computational Sciences and Technology

**Stanford University**  
**Program:** Institute for Computational and Mathematical Engineering (ICME)

**State University of New York Brockport**  
**Program:** Computational Science  
**Program Description:** 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.

**State University of New York Stony Brook (SUNY/SE)**  
**Program:** Computational Applied Mathematics Program

**Technische Universität München**  
**Program:** Computational Science in Engineering  
**Degree:** Master's degree in Computational Engineering

**Technische Universität Braunschweig**  
**Program:** Computational Science in Engineering  
**Degree:** Bachelor's and Master's degrees

**Universität Erlangen-Nürnberg**  
**Program:** Computational Science and Engineering  
**Degree:** Bachelor's and Master's degrees

**University of California, Santa Barbara**  
**Program:** PhD in Applied Mathematics with a Computational Mathematics Option

**University of Colorado, Denver**  
**Program:** Graduate Program in Scientific Computation

**University of Delaware**  
**Program:** Computational Sciences Program  
**Degree:** Interdisciplinary graduate certificate program

**University of Houston**  
**Program:** Computational Science and Applied Mathematics  
**Degrees:** PhD in Mathematics with Major in Computational Science cluster of Mathematical Computer Science program or any cluster in Applied Math program

**University of Illinois, Chicago**  
**Program:** Computational Science and Engineering (CSE)  
**Option:** MS and PhD in Participating Depts with Minor Certificate in CSE

**University of Illinois, Urbana**  
**Program:** Computational Science and Engineering (CSE)  
**Degree:** PhD in Mathematical Sciences

**University of Iowa**  
**Program:** Applied Mathematics and Computational Sciences Program  
**Degree:** PhD in Interdisciplinary AMICS Program

**University of Iowa**  
**Program:** Applied Mathematics and Computational Sciences Program  
**Degree:** PhD in Interdisciplinary AMICS Program

**University of Manchester**  
**Program:** MSc in Computational Science

**University of Michigan**  
**Program:** Doctoral Program in Scientific Computing  
**Certificate:** Certificate in scientific computing appended to departmental degrees

**University of Minnesota**  
**Program:** Scientific Computation Program  
**Degrees:** MS and PhD in Scientific Computation

**University of Oxford**  
**Program:** MSc degree in Mathematical Modelling and Numerical Analysis, D. Phil degree in Numerical Analysis

**University of Southern Mississippi**  
**Program:** Scientific Computing

**University of Texas, Austin**  
**Program:** Texas Institute for Computational and Applied Mathematics (TICAM) Program  
**Degrees:** MS and PhD in computational and applied mathematics

**University of Utah**  
**Program:** Computational Engineering & Science Graduate Program (CEGSP)

**Uppsala University**  
**Program:** Department of Scientific Computing

**William and Mary**  
**Program:** Graduate Studies in Computational Science, Studies in computer science cluster leading to certificate

### Computational Finance

**Carnegie Mellon University**  
**Program:** MS in Computational Finance

**Cornell University**  
**Program:** Financial Engineering Option

**Columbia University**  
**Program:** Masters Program in Financial Engineering

**Purdue University**  
**Program:** Computational Finance Program

**University of Chicago**  
**Program:** Master of Science in Financial Mathematics

**University of Nijmegen**  
**Program:** MS in Financial Engineering

**University of Toronto**  
**Program:** Mathematical 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 (CalS).
    - 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 CalS 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)
# How It Might Work For Students

<table>
<thead>
<tr>
<th>Degree Program</th>
<th>Recognition Sought</th>
<th>Requirements</th>
</tr>
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<tbody>
<tr>
<td>Master’s in Home Dept.</td>
<td>Minor in Computational Science</td>
<td>9 hrs.: 6 @ level A, 3 @ level B</td>
</tr>
<tr>
<td>Doctorate in Home Dept.</td>
<td></td>
<td>15 hrs.: 6 @ level A, 9 @ level B</td>
</tr>
</tbody>
</table>

- 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.