Graduate Concentration in Computational Science University of Tennessee, Knoxville

Program Description

What is Computational Science

Many of the outstanding problems in science and engineering today are so computationally challenging that a new scientific approach is required in order to solve them. 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, which is at the foundation of the field of *Computational Science*, 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 is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems. Computational science fuses three distinct elements: (a) mathematical modeling of the phenomena being studied, translation of these models into computational processes via step-by-step algorithms (both numerical and non-numerical), and development of application software that encodes the models and algorithms to solve problems in the sciences, engineering, and the humanities; (b) computer and information science that develops and optimizes the advanced system hardware, software, networking, and data management components needed to run these complex and resource intensive scientific applications; and (c) the actual computing infrastructure necessary to support the other two elements.

Computational science provides an essential complement to experimentation and theory in several different ways. First, it often enables problems to be solved more efficiently, more rapidly and less expensively. Second, it can solve problems computationally that otherwise could not be solved safely. Finally, it can solve problems whose solution would otherwise be impossible (e.g., due to the overwhelming amount of data involved or to an inability to recreate experimental conditions).

Our interest in computational science reflects the large, sustained, and widespread growth in this multidisciplinary area. As distinguished from traditional Computer Science, *Computational Science* is a field that studies a new class of science and engineering problems, the solution to which depends on the *combination of* state-of-the-computer science *and* domain-specific expertise in such areas as Physics, Chemistry, Medicine, Engineering, Biology, and Geology. But since it requires the *recombination* of knowledge, skills, and expertise across the boundaries of traditional academic domains, developing academic programs that prepare students for its demands represents a significant challenge.

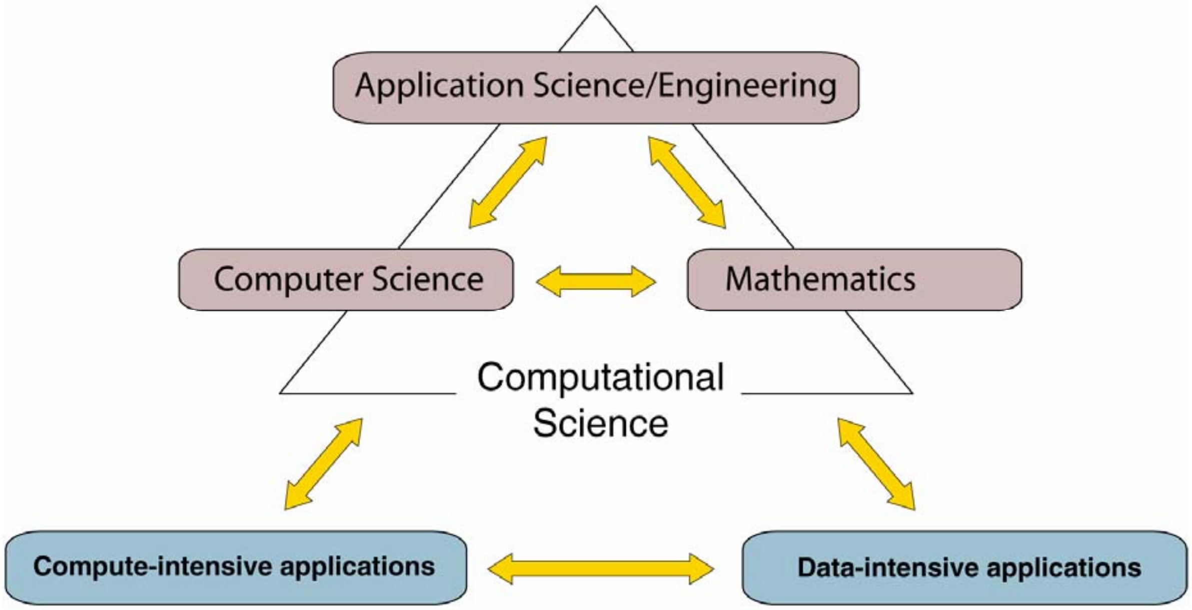

Figure 1: Relationships between Computational Science, Computer Science and Applications

Substantial growth in computational science at Tennessee has arisen through the world-leading efforts of several multidisciplinary research and education initiatives, including Oak Ridge National Laboratory, the Innovative Computing Laboratory, the Institute for Environmental Modeling, UT-ORNL Graduate School of Genome Science & Technology, the Joint Institute of Computational Sciences, the Joint Institute of Biological Sciences, as well as others.

The effects of such growth are not isolated but rather have enormous positive impact on the community as a whole, an impact that extends far beyond the infusion of millions of research dollars annually into the Tennessee economy. Many of us on the faculty are already working in rich, interdisciplinary collaborations with researchers at other universities, in industry, at the national laboratories and healthcare institutions across the nation. These collaborations are necessary to attack complex multidisciplinary problems that can combine elements from a highly diverse collection of different fields, such as geophysics, chemical engineering, molecular dynamics, aerospace fluid mechanics, combustion, atmospheric dispersion, nano-science, earth and planetary studies, robotics, cardiology, radiology, neurology, and small animal imaging.

Computational Science as an emerging academic pursuit

The rapid emergence of the computational science paradigm is already having a profound effect on the needs and aspirations of our faculty, our students, and the industries and businesses in our state. There is a growing need to complement current graduate programs with programmatic efforts that reflect the breadth and the multidisciplinary nature of this new research methodology. In order to address this critical challenge, the proposed graduate degree concentration in Computational Science is designed to complement existing multidisciplinary programs in areas such as Computer Science, Mathematics, Physics, Chemistry, Biological Sciences, and Engineering. Until we can put into place the educational programs that will permit this training to occur, the scientists and engineers we help to produce will not be able to fulfill their potential and Tennessee will not realize the highest return on its investment.

To understand why this movement is expanding so quickly in the US and Europe, and why it demands leading edge computer science combined with domain-specific expertise, one only needs to consider the kinds of questions it aims to address. Examples of such problems include the following:

- How can we efficiently store, model, visualize and understand the mass of data generated by the human genome program?
- How might we digitize patient records such that they help medical practitioners rather than drown them in a mass of irrelevant data and baroque procedures?
- How can we model disease transmission in populations that are structured in complicated ways, such as the vectors of the West Nile virus?
- How can we use the extraordinary amount of information recorded by point-of-sale checkout machines to better coordinate retail industries with the shoppers that drive them?
- How might software agents be built such that we trust them to do our shopping online?
- How might we model, simulate and visualize the functions of the heart and brain to better diagnose and treat cardiac and neural abnormalities with a view to improving the quality of life?
- How might we compute solutions to realistic physical models of dangerous situations such as explosions with a view to improving safety?

The next wave of industry growth will focus on business opportunities resulting from the answers to questions such as these. The faculty in the Colleges of Arts and Science and Engineering (CoAS/CoE) are already performing research that embodies the multidisciplinary computational methods that these questions demand. This proposal for new graduate program in Computational Science seeks to provide an academic program that encapsulates the pursuit of these challenges into a marketable credential for Tennessee students.

Two key features of the proposed Computational Science degree structure are particularly designed to meet the student's expectation. First, the new Computational Science concentration is designed to integrate knowledge from many starting points (engineering, mathematics, physics, medicine), and thus offers students the opportunity to enter the program through a variety of different doors. Second, its track structure makes it possible to build natural and student-centered collaborative academic programs across the University, enhancing the kind of cross fertilization of ideas on which original research thrives.

<u>Managing a multi-disciplinary program</u>

The proposed graduate concentration structure will operate at both the Masters and Doctoral level and will be interdisciplinary through its track structure. Each track will have a group of faculty members who will form a Track Faculty Committee or TFC (these will most likely be from a specific department). The TFC will, in collaboration with the Director of the Joint Institute for Computational Science (JICS), be responsible for the creation and subsequent administration of a track. This track structure will make it possible for the graduate concentration to be applicable to emerging multidisciplinary problems with a maximum of efficiency in a sound academic manner. We note that academic tracks have been shown to be a successful mechanism for offering a variety of educational opportunities within a larger degree option.

Examples of possible academic tracks formed under the umbrella of the computational science concentration include:

(i) Scientific Computing
(ii) Scientific Imaging and Visualization
(iii) Applied Combinatorics
(iv) Software Engineering
(v) Computational Robotics
(vi) Genome Sciences
(vii) Earth and Planetary Science

A key role of the TFC will be to ensure that the track has academic standards consistent with and as academically rigorous as those of the participating departments, schools or institutes at both the masters and doctoral level. The degree itself will be awarded within the department that the student is enrolled.

The degree concentration will create a balance between traditional Computer Science and problem-specific content in the training tailored to the common needs of the students and the and the academic disciplines involved in the multidisciplinary application area. Our administrative plan follows a common format used by many programs that are organized into tracks.

Computer Science MS and PhD with Concentration in Computational Science:

- Students in this program must take CS530 plus two of CS560, CS571, CS580, or CS581.

- MS students must take min 3/max 6 hrs of non-CS listed 500-level or 600-level course work from a different academic unit, eg math, physics, or geology. The specific courses must be approved by both the student's committee and the CS graduate committee.

- MS students must do a thesis. The committee consists of at least three people: chair and one more member from CS plus a person affiliated with JICS.

- PhD students must take min 6/max 12 hrs of non-CS listed 500-level or 600-level course work from a different academic unit, eg math, physics, or geology. The specific courses must be approved by both the student's committee and the CS graduate committee.

- MS and PhD students are encouraged to seek an internship at least once thru the CS592 mechanism.

- The PhD Comp. Exam is changed to accommodate the above change in what we consider to be core courses.

- A PhD committee consists of at least five people: chair and one more member from CS, a member from a different academic unit, plus a person affiliated with JICS.

Engineering Science Graduate Program - Catalog Revisions 2005

Certificate in Computational Fluid Dynamics

The College of Engineering offers a certificate program in computational fluid dynamics through the Engineering Science graduate curriculum. The program is designed principally for working professionals, as enabled by the course content being completely available at a distance via the Internet venue.

The 12-hour certificate is initialized by completing ES 551, Computational Engineering Sciences, and ES 552, Computational Fluid Dynamics, both 3 credit hours. These courses are cross-listed with participating departments in the College. Certificate program completion is via two elective courses, selected from those listed as available at the UT CFD Laboratory website (cfdlab.utk.edu). Courses currently available include ME 452, Finite Element Analysis, ChE 507, Matrix Methods in Engineering, and ES 645, Advanced Topics in Turbulence. Additional elective courses will become available as this certificate program matures. Participants must make application and be admitted to the Graduate School.

Chemical Engineering Graduate Program – Concentration in Molecular-Level Simulation

The Department of Chemical Engineering offers a concentration program in molecular-level simulation through the Chemical Engineering graduate curriculum. The program is designed principally for onsite graduate students. The 12-hour concentration is initialized by completing:

- Advanced Mathematics for Engineers ChE/MSE 505,
- Transport Phenomena II, ChE 548
- Statistical Mechanics, ChE 532 or

concentration program completion is via one elective course, to be approved by the concentration committee. Courses currently available include Statistical Mechanics II (ChE 631) and Special Topics in Simulation (ChE 691). Additional elective courses will become available as this concentration program matures. Participants must make application and be admitted to the Graduate School.

Department of Geography Graduate Concentration in Computational Science:

The Department of Geography offers a graduate concentration program in computational aspects of geographic information science. This graduate concentration program requires a minimum of 12 credit hours as listed below.

Required Courses (6 credit hours):

- Geography 510 - Geographic Software Design
- Geography 517 - Geographic Information Management and Processing
- M.S. and Ph.D. students are encouraged to take an up to 6 hours of internship through Geography 519 with the Geographic Information Science and Technology Group at Oak Ridge National Laboratory or other organization approved by the Department

Elective Courses (6 credit hours): (choose two courses from the list below)

- Geography 513 - Topics in Remote Sensing
- Geography 518 - GIS Project Management
- Geography 549 - Topics in Transport Geography
- GIScience seminar

Prerequisite:

- Geography 411 – Computer Mapping and Geographic Information Systems (or equivalent)

Department of Mathematics Graduate Concentration in Computational Science:

The Department of Mathematics offers a concentration program in Computational Science. The program is designed for M.S. or Ph.D. level graduate students from any department, or professionals with a graduate degree, who desire a background in Computational Science.

The 21-credit concentration requires that a student complete:

- 2 courses in modeling, chosen from Math 475 or 578, 513 or 537, 581;
- 2 courses in computational methods, chosen from Math 572 or 574, 577, or Stat 571;
- 2 courses from an area outside of mathematics. These courses are to be chosen in consultation with the Track Faculty Committee (TFC) of the Mathematics Department.
- 3 credits of Math 500 to complete a computational science project under the supervision of a faculty member and approved by the TFC.

School of Information Sciences Graduate Concentration in Computational Science: Human Computer Interaction (HCI)

This track focuses on the human and social dimensions of computer system design and use with two strands of emphasis: (1) the novel interaction between people and computers beyond conventional desktop computing; and (2) the role that computer systems can play in collaborative work between individuals, groups, and organizations. Topics associated with HCI include: adoption and diffusion of collaborative technologies; software architectures for user-adaptive systems; universal access to interactive systems;
Design principles for information visualization; and new patterns of computer-mediated work such as virtual teams.

Course Requirements:

- IS 588 *Human-Computer Interaction*
- IS XXX *Information Visualization* (a new course)
- Psy 453 *Cognitive Science*
- CS 525 *Software Engineering* or CS 594 *Graphical User Interfaces*

School of Information SciencesGraduate Concentration in Computational Science: Knowledge Mining

The rapid growth of computer-based information systems and their global interconnectivity has resulted in a severe information overload in all areas of science and technology. This problem is accelerating with the expansion of the internet and related technologies. The graduate certificate in knowledge mining focuses on the methods and tools for assisting scientists, researchers and other professionals in the effective extraction of problem-oriented knowledge from diverse and massive information sources, and for using this knowledge in problem solving situations. Emphasis is given to novel and creative methodologies that generate knowledge through inference from data and information, and present the generated knowledge in user-oriented forms.

Course Requirements:

- IS 584 *Database Management Systems*
- IS XXX *Information Visualization* (a new course)
- Stats 571 *Statistical Methods*
- CS 594 *Advancements in Data Mining*

Department of Animal Science MS and PhD with Concentration in Computational Science:

- Student must satisfy all requirements of the Animal Science Degree program.

- Student's graduate committee must have one member from the Computer Science department or a JICS faculty member.

- Students must take CS471-CS472 and CS571-CS572.

- At least one chapter of the thesis or dissertation should be focused on a problem that uses scientific computing approaches.

- Students are encouraged to seek internship or special problem opportunities to complement the above requirements.

Department of Physics MS and PhD with Concentration in Computational Science:

- The standard core curriculum: Physics 521-522, 531, 541, 551, and 571 (18 hours).

- Additional mathematical, numerical, and computational courses in the Physics Department: Physics 572, 573, and 643 (9 hours).

- Numerical Mathematics: CS/Math 571-572, for which the above will hopefully provide satisfactory prerequisites (6 hours).

- An additional course at the 500 level, either in the Physics and Astronomy department, or if approved by the student’s committee and the graduate committee, another relevant academic unit (e.g. Computer Science, Mathematics, Information Science) (3 hours).

- Two 600-level Physics courses in the cognate field to which computational methods will be applied in doctoral research (atomic physics, nuclear physics, elementary particle physics, astrophysics, etc.) (6 hours).

- Two additional courses at the 600 level, either in the Physics and Astronomy department, or if approved by the student’s committee and the graduate committee, another relevant academic unit (e.g. Computer Science, Mathematics, Information Science) (6 hours).

- 24 hours of Doctoral Research and Dissertation (Physics 600), which shall involve computational methods in a significant way.

Note that in addition to the 18 hour core, these specifications include 15 hours at the 500 level and 15 hours at the 600 level. The deviations from the standard department requirements are specification of 15 hours of particular coursework (points 2 and 3 above), and allowance (with approval) for up to 9 additional hours outside the department (points 5 and 6).

Other departments would list their concentration in Computational Science here

Appendix:

Definition of a Graduate Certificate Program

From page 27 of the 2004-2005 University of Tennessee Graduate Catalog, (see http://diglib.lib.utk.edu/dlc/catalog/images/g/2004/g_1.pdf).

Graduate Certificate Programs

A graduate certificate may be earned by successful completion of a series of specific courses. A candidate for a graduate certificate program must be a fully admitted graduate student who has satisfactorily completed (minimum 3.0 grade point average) the minimum requirements for certificate programs are listed under the academic department offering the certificate. A candidate must be a graduate student in good standing and comply with all other applicable policies. Graduate certificate programs require a minimum of 12 semester credit hours taken at the University of Tennessee, Knoxville. Use of credits to fulfill requirements for a graduate degree will be at the discretion of the academic department. To receive the certificate, students must submit an application endorsed by the academic department to the Office of the University Registrar. Only those certificate programs that are officially approved by the Graduate Council will be posted on student transcripts. To receive a graduate certificate, students must be admitted to a certificate program or a degree program.

Here is a quick summary of the essential difference between a Certificate and a Concentration:

- Certificate: A certificate, roughly speaking, is a kind of "half masters" in a given area, i.e. it requires something like 15 hours of course work in that area. It may be hosted by a given department, but it is outside their normal degree programs. Any student at the University, regardless of the degree program they're in, can earn the certificate if they can do the work, and they can get the certificate whether or not they get a degree.

- Concentration: With a concentration in Computational Science, each participating department would, upon the student's completion of additional academic work, grant a degree in their field "with a concentration in Computational Science." Computational Science concentrations would add value to the degrees that departments are already granting, which makes them easier to understand and easier for departments to support.

Distribution:

In an attempt to use the broadest use of computational science and reach as many as possible this information has been sent to the following people:

Faculty in departments with a presumed interest in seeing a "Computational Science Concentration" succeed at the University of Tennessee

Department	First name	Last name
Mathematics	Vasilios	Alexiades
Industrial and Information Engineering	Adedeji	Badiru
Engineering Science	A.J.	Baker
Microbiology	Jeffrey	Becker
Theory and Practice in Teacher Education	Susan	Benner
Veterinary Medicine	Michael	Blackwell
Economics	Robert	Bohm
Statistics, Operations and Management Science	Ham	Bozdogan
Materials Science & Engineering	Ray	Buchanan
University Outreach & Continuing Education	Norvel	Burkett
Dean Arts and Science	Bruce	Bursten
Physics	Chritian	Cardall
Chemical Engineering	John	Collier
Civil & Environmental Engineerin	Chris	Cox
Dean's A&S Office	Don	Cox
Chancellor	Loran	Crabtree
Nursing	Joan	Creasia
Journalism & Electronic Media, School of	James	Crook
Small Animal Clinical Sciences	Robert	DeNovo
Exercise, Sport and Leisure Studies	Joy	DeSensi
Libraries	Barbara	Dewey
History	Todd	Diacon

Nuclear Engineering	Harold	Dodds
Computer Science	Jack	Dongarra
Dean's office A&S	William	Dunne
Electrical & Computer Engineering	Samir	El-Ghazaly
Consumer Services Management	Nancy	Fair
Political Science	David	Feldman
Instructional Technology and Educational Studies	Russell	French
Sociology	R. Scott	Frey
Law	Tom	Galligan
Large Animal Clinical Sciences	Dennis	Geiser
Health and Safety	Thomas	George
Food Science & Technology	Charles	Goan
Computer Science	Jens	Gregor
Ecology & Evolutionary Biology	Louis	Gross
Biochemistry, Cellular and Molecular Biology	Hong	Guo
Communication Studies, School of	John	Haas
Philosophy	John	Hardwig
Chemistry	Robert	Harrison
Chemistry	Robert	Hinde
Forestry, Wildlife and Fisheries	George	Hopper
Department of Industrial & Information Engineering	Myong	Jeong
Entomology & Plant Pathology	Carl	Jones
Management	William	Judge
Communication and Information	Faye	Julian
Agricultural Sciences and Natural Resources and Tennessee Agricultural Experiment	Thomas	Klindt
Anthropology	Andrew	Kramer
Dean Engineering	Way	Kuo
Psychology	James	Lawler
Department of Industrial & Information Engineering	Xueping	Li
Art	Sarah	Lowe
Educational Psychology and Counseling	Steve	McCallum
Earth and Planetary Sciences	Harry	McSween
Modern Foreign Languages & Literatures	Jeff	Mellor
Dept. of Earth and Planetary Sciences	Jeffrey	Moersch
Earth and Planetary Sciences	Claudia	Mora

Accounting and Information Management	Daniel	Murphy
Comparative Medicine	John	New
Child and Family Studies	Vey	Nordquist
Agricultural Economics	Charles	Norman
Physics	Thomas	Papenbrock
Engineering Fundamentals	J. Roger	Parsons
Microbiology Department	Cynthia	Peterson
Science Alliance	Jesse	Poore
Geography	Bruce	Ralston
Plant Sciences	G. Neil	Rhodes
Education, Health, and Human Sciences	Robert	Rider
Architecture, School of	Max	Robinson
Theatre	Blake	Robison
Animal Science	Arnold	Saxton
Botany	Edward	Schilling
Religious Studies	Gilya	Schmidt
Pathobiology	Hildegard	Schuller
Audiology and Speech Pathology	Ilsa	Schwarz
Architecture & Design	Jan	Simek
Social Work	Karen	Sowers
Music	Roger	Stephens
Classics	David	Tandy
Advertising and Public Relations, School of	Ron	Taylor
Information Science	Carol	Tenopir
Interim Vice President of Research	Fred	Tompkins
Information Science	Peiling	Wang
Finance	James	Wansley
Biosystems Engineering & Environmental Science	Tristram	West
Nutrition	Jay	Whelan
Business	Jan	Williams
Marketing and Logistics	Robert	Woodruff
VP Research	Clif	Woods
Associate Lab Director ORNL	Thomas	Zacharia
Microbiology	Igor	Zhulin
English	John	Zomchick

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