Proposal to Establish a Ph.D. in Computational Science

Middle Tennessee State University

FORM - COVER

Sponsoring Institution(s): Middle Tennessee State University

Proposal: Doctor of Philosophy in Computational Science

Degree Designation [or] Type of Certificate:

Ph.D. in Computational Science.
Formal Degree Abbreviation — Title of Proposed Program to be established or impacted

Concentrations: N/A

Delivery Site(s): Middle Tennessee State University

Proposed CIP Code:

Proposed Implementation Date: Fall 2009

Cooperative Partners: N/A

For more information contact: Dr. Michael Allen / 615-898-2840.
Name — Telephone

Institutional Approval:___________________________/______
Signature of President ***Date***

FORMAT - SUM (Summary)

INSTITUTION: Middle Tennessee State University

PROPOSAL: Doctor of Philosophy in Computational Science

EFFECTIVE DATE: Fall 2009

PURPOSE (Goals and Objectives):

The Ph.D. in Computational Science at MTSU seeks to create a strong research-centered degree program in which faculty from biology, chemistry, computer science, mathematical sciences, and physics and astronomy will collaborate to teach and train a new generation of graduates skilled in a computational approach to scientific investigations.

The proposed Ph.D. degree will use computational science as the nexus drawing together a multidisciplinary cross section of research-active faculty from the College of Basic and Applied Sciences to provide unique educational and research opportunities centered on numerical solution, computational modeling, and computer simulation of complex problems. The aim of the Computational Science Ph.D. at MTSU is to produce graduates with competency in the following three key areas:

- mastery of the mathematical methods of computation as applied to scientific research investigations coupled with a firm understanding of the underlying fundamental science in at least one disciplinary specialization;
- deep knowledge of programming languages and computing technology so that graduates can adapt and grow as computing systems evolve; and
- skills in effective written and oral communication so that graduates are prepared to assume leadership positions in academia, national labs, and industry.

The aim of the Computational Science Ph.D. is to be research intensive and applied. From the beginning of their time on campus, students will be involved in research groups and exposed to the breadth of interdisciplinary problems being addressed by individual faculty members and their collaborations. A key goal of the coursework and the early involvement in research is to help students achieve a broader view of computational science as an approach that can be applied within and across traditional disciplines. The combination of interdisciplinary research exposure and a core curriculum created to develop scientific knowledge and communication skills is consistent with the philosophy of the nationally recognized "Preparing Future Faculty" program (*www.preparing-faculty.org*), the "Reshaping the Graduate Education of Scientists and Engineers" report of the National Academy of Sciences (*www.nap.edu/catalog/4935.html*), and the model Ph.D. programs proposed by NSF through its funding program entitled "Integrative Graduate Education and Research Traineeship Program" (IGERT; *http://www.igert.org/*). Graduates of the Ph.D. in Computational Science will be prepared with a unique mix of skills that will permit them to pursue research careers in academia, government, and industry laboratories.

CURRICULUM: The proposed program requires completion of 72 semester credit hours distributed as follows:

Curriculum Component	Hours Required
Core Courses	
Foundation courses	9
Computational Science Core	36
Electives	15
Dissertation	12
TOTAL:	72

No. of new courses: 19 with 58 credit hours

NEED:

High-speed computing has revolutionized the manner in which knowledge is acquired in almost every discipline of science. Occupying a position between theory and experiment, computational science—often referred to as the 'third pillar' of scientific inquiry—provides a methodology to seek solutions to problems that are insoluble or impractical by traditional techniques. The ability of computational science to model and visualize complex systems is generating fresh knowledge that crosses traditional discipline boundaries. As described in the reports cited in the Performance Justification section below, the national need for skilled graduates in computational science is well established. Furthermore, computational science—particularly of the form being proposed here—fits well with current science and areas of business growth within the State of Tennessee. Computational science is one of the six research and development emphasis areas selected by the Tennessee EPSCoR Committee in 2003-2004 (*https://my.tennessee.edu/portal/page?_pageid=37,1&_dad=portal&_schema=PORTAL*).

IMPACT:

Computational science is critical to scientific excellence, economic competitiveness, and national security. This degree program will increase the availability of highly-trained computational scientists with strong applied technical skills and a broad interdisciplinary research perspective. Skilled graduates will enhance the academic and economic well being on both the state and national levels. In the process, the program will expand MTSU's contribution to original scholarly research in the area of computational science.

PLANS FOR ACCREDITATION: N/A

ATTACHMENTS: N/A

FORMAT - PS (Program Structure)

A. **Total Credits Required for Graduation:** 72 credit hours post-baccalaureate*

* Students entering with a master's degree in a mathematics, science, or engineering discipline may apply up to 12 graduate hours from a previous graduate degree to the 72 hour requirement, after determination that the content of the courses is directly equivalent to existing courses in the Computational Science curriculum. This assignment is made at the recommendation of the Program Coordination Committee and with the approval of the graduate dean.

B. Residency requirements (if any):

All students in the Computational Science Ph.D. Program will be expected to complete a minimum of two consecutive semesters of full-time study in residence at MTSU. This program only accepts full-time students.

C. Core Courses: Total credits: 39 hours

The computational science foundation courses are designed to take students from diverse majors and prepare them to successfully enter the computational science core. The computational science core is designed to give students a thorough grounding in the fundamental tools and methods necessary for a research career in computational science. The core courses are sequenced so as to prepare students to take the elective courses.

Foundation Courses – 9 credit hours		
COSC 6100	Fundamentals of Computational Science	3 credits
MATH 6500	Fundamentals of Scientific Computing	3 credits
CSCI 6300	Fundamentals of Programming Languages	3 credits
Computational Science Core – 30 credit hours		
COSC 7800	Teaching Internship	3 credits
COSC 7950	Research Seminar in Computational Science	2 credits
CSCI 7500	Databases and Visualization	4 credits
CSCI 7200	Scientific Programming	4 credits
MATH 7300	Numerical Methods	3 credits
MATH 7400	Computational Statistics	3 credits
MATH 7800	Parallel Computing	4 credits
MATH 7100	Applied Computational Science	4 credits
MATH 7750	Mathematical Modeling	3 credits

D. Electives: Total credits: 15 hours

In consultation with the major professor and the dissertation committee, the student: • *Must take a minimum of 15 hours of 6000/7000 credit within science departments;* • *Must select 3 courses from the following list;*		
MATH 6720	Advanced Differential Equations	3
MATH 6300	Optimization	3
MATH 7450	Mathematical Models in Biology	3
CHEM 7720	Advanced Topics in Physical Chemistry	3
CHEM 7400	Computational Chemistry I	3
CHEM 7410	Computational Chemistry II	3
PHYS 7400	Computational Physics I	3
PHYS 7410	Computational Physics II	3
BIOL 6450	Advances in Molecular Genetics	3
BIOL 6366	Biostatistical Analysis	3
BIOL 6390	Advanced Cell/Molecular Biology	3
BIOL 6760	Bioinformatics	4
BIOL 7400	Computational Biology I	3
BIOL 7410	Computational Biology II	3
CSCI 6100	Analysis of Algorithms	3
CSCI 6130	Topics in Parallel Processing	3
CSCI 7350	Data Mining	3

E. Directed Research: Total Credits 6 hours

Students will complete a minimum of 6 credit hours of directed research in Computational Science prior to advancement to candidacy.

COSC 7900	Directed Research in Computational Science (6 hours needed before candidacy)	1-6 credits, 6 total

F. Research/Dissertation: Total Credits 12 hours

Every student in the proposed Ph.D. in Computational Science will be required to undertake, complete, and successfully defend a dissertation which will be interdisciplinary in nature. Students are only allowed to enroll in Dissertation Research following their advancement to candidacy after successful completion of a qualifying exam.

COSC 7640	Dissertation Research (minimum 12 credits required.)	1-6 credits

G. Admission, Retention, and Graduation Requirements:

The program will be constituted in accordance with the existing university requirements described in the Graduate Catalog.

Proposed Catalog Description of Admissions Requirements

Admissions are based on a comprehensive assessment of a candidate's qualifications including Graduate Record Examination (GRE) test scores, undergraduate and graduate grade point average, and letters of recommendation. Applicants must:

1. Formally apply for admission to the College of Graduate Studies and fulfill all requirements, including submission of official transcripts from all academic work and official scores on the Graduate Record Examination.

2. Hold a baccalaureate, master's, or doctoral degree in a science discipline. Applicants holding a master's degree will be expected to have earned at least 21 semester hours of graduate mathematics, science, or engineering credit, with evidence of strong mathematical skills and experience in computation through coursework, employment, and/or research experiences. Students entering with a master's degree in a mathematics, science, or engineering discipline may, on the recommendation of the program coordination committee and with the approval of the graduate dean, have up to 12 credit hours accepted from their master's if it directly corresponds to coursework in the Computational Science curriculum. Applicants applying from the baccalaureate level must have an appropriate science degree with evidence of strong mathematical skills and experience in computation through coursework, employment, and/or research experiences. Applicants lacking necessary foundational coursework in previous degrees will be required to complete these courses as part of their program of study in addition to the degree requirements. In addition, students admitted to the computational science program will be required to participate in an intensive computational science leveling program prior to the beginning of their coursework.

3. Have a grade point average (GPA) in previous academic degrees which indicates potential for success in advanced study. Successful applicants typically present a minimum 3.5 GPA in their master's degree or a minimum 3.0 GPA when entering with a bachelor's degree.

4. Submit scores for the verbal, quantitative and analytical writing measures of the Graduate Record Examination (GRE) that indicate potential for success in the Computational Science program. The GRE is an important measure and is given significant consideration in the admissions review process. Successful applicants typically have scores on the Verbal and Quantitative measure at or above the 50^{th} percentile for persons intending graduate study in science with a combined V + Q score that exceeds 1000.

5. Provide letters of recommendation from at least three professors or professionals that address the applicant's potential to successfully complete a Ph.D. in the computational science program.

6. International students must also meet the College of Graduate Studies requirement for proof of English language proficiency. This may be accomplished by

submission of TOEFL, UMELI test, or IELTS scores that meet CGS requirements, or by successful completion of level 112 of ELS coursework.

Applicants who do not meet these minimums but whose application materials indicate high potential for success may be admitted conditionally and would have to meet the conditions of their admission in the time stated to remain in the program of study.

Additional Application Information

The application deadline is February 15 for those wishing to be considered for graduate assistantships for the following fall. Late applications may be considered but admission and financial support in the form of an assistantship is not guaranteed.

Retention and Graduation Information

Students must meet the expectations of the university as regards adequate progress toward the degree. Specifically:

1. Doctoral students are expected to maintain a 3.25 grade point average for all graduate coursework.

2. Students may not enroll in more than one semester before full admission is granted.

3. Students must complete and submit an Advancement to Candidacy form by the time two semesters are completed.

4. Students are expected to consistently enroll in and complete coursework in their area of study, making continuous progress toward attainment of the degree.

5. Once admitted to candidacy and enrolling in dissertation (COSC 7640), students are expected to maintain continuous enrollment.

6. At least two thirds of the credits counted toward the degree must be at the 7000 level.

Additional Graduation Requirements

Because the aim of the Computational Science Ph.D. is to produce students who are fully prepared to pursue research careers in academia, industry, and at national labs, the Computational Science Ph.D. program will put in place a series of benchmarks to be accomplished as the student progresses along the path to graduation. The benchmarks fall into three specific categories. Students must:

1. Make at least two research presentations at regional, national or international meetings as the lead or co-author.

2. Be lead author or make significant contribution as co-author of two articles published, in press, or under review in high-quality peer-reviewed journals.

3. In collaboration with an MTSU faculty member serving as principal investigator, make a significant contribution to the development of at least one external grant proposal.

Although some of these expectations would be realized naturally in the course of a student's progress towards the Ph.D., the Computational Science program at MTSU makes them explicit to emphasize to incoming students the expectation that they will become active and engaged participants in the research process. Publications and presentations are already recognized as standard metrics of research progress. The involvement of Ph.D. students in the grant writing process is a developing trend designed to train graduates to be more effectively prepared for jobs in the research environment. Experience in grant writing is both a necessary skill and an important insight into the manner in which science and engineering are funded. Because grant agencies require the principal investigator (PI) to have a permanent academic position, the grant will be written as a collaboration with the major professor who will serve as the PI.

A student's progress on the benchmarks will be reviewed annually with his or her adviser or dissertation committee. The projected timeline on these benchmarks would be that presentations would be a real possibility beginning early after candidacy. The grant authorship and publications would normally occur later in a student's research program as evidence of his/her ability to contribute at the highest level of computational research.

H. Describe any unique features such as interdepartmental cooperation, collaboration with other institutions, articulation, industry partnerships, etc.

The Ph.D. in Computational Science at MTSU will be based on interdepartmental cooperation, utilizing, as it will, faculty from biology, chemistry, computer science, physics and astronomy, and mathematical sciences. Computational science, by its nature, looks at problems that cross traditional disciplinary boundaries. This modern, broad-based approach to science will be inculcated in our students by their participation in interdisciplinary research groups and an emphasis on dissertation research problems that straddle traditional disciplines. In addition to interdisciplinary research, all candidates will experience a common science core of coursework and seminars, and a mandatory teaching experience. The combination of interdisciplinary research and a balanced curriculum will enable graduates of the Ph.D. in Computational Science to be well-trained with technical, professional, and communication skills and a deep knowledge in their chosen disciplines.

MTSU signed a Memorandum of Understanding (MOU) with Oak Ridge National Laboratory (ORNL) and is a member of the Oak Ridge Associated Universities (ORAU).

ORNL is home to the National Center for Computational Sciences which provides the most powerful computing resources in the world for open scientific research. As part of the MOU, computational scientists at ORNL have agreed to make the computing resources and expertise of the laboratory available to MTSU Computational Science Ph.D. students. MTSU Computational Science Ph.D. students will spend time on site at ORNL and will make use of the super-computers at ORNL for their research. The growing relationship with ORNL has already led the faculty in the Computational Science program to work on joint projects and to apply for joint funding with scientists at ORNL. The connection to ORNL's world class facilities, expertise, and reputation in computational science will be a significant factor in ensuring the success of the Computational Science Ph.D. at MTSU.

Interdisciplinary Nature of the Degree

"Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation. Advances in computing and connectivity make it possible to develop computational models and capture and analyze unprecedented amounts of experimental and observational data to address problems previously deemed intractable or beyond imagination." (report of the President's Information Technology Advisory Committee (PITAC), June 2005)

Computational science as a discipline does not have its own set of problems to solve. The problems that computational scientists address are interdisciplinary in nature and are drawn from the life and physical sciences, including biology, chemistry, physics, engineering, and environmental science. With a strong set of computational skills developed by taking the foundation and core coursework, the Computational Science graduate students will be capable of addressing complex interdisciplinary problems that cannot be understood through the other two pillars of scientific discovery; theory and experimentation.

The interdisciplinary objectives of the program are addressed within the university in several ways.

1. Curriculum. The curriculum includes formal coursework in several traditional disciplines in the sciences. These include biology, chemistry, mathematics, computer science, and physics and astronomy. A Program Coordination Committee (composed of graduate coordinators from each participating department) will have primary responsibility for reviewing the proposed course sequence for each student, ensuring that this curriculum is well-integrated and coherently focused on topics that satisfy the broad educational and research goals of the program.

2. Program Coordination Committee. Primary responsibility for the coherence of the curriculum lies with the Program Coordination Committee (PCC). The dean of the College of Basic and Applied Sciences is responsible for selecting and appointing

participating graduate faculty members to serve on the PCC from the program faculty holding doctoral level graduate faculty membership and for ensuring the coherence of (and adherence to) the program's curriculum.

3. Colloquia/Symposia. The program will hold regularly scheduled colloquia and symposia. These colloquia/symposia will be presented in a variety of formats: individual presentations of research findings and policy positions; debates; panel discussions; and topical forums. These events make a significant contribution to the educational content of the program in addition to building a sense of community among the science Ph.D. students. In addition to faculty presenters, invited presenters will include local and visiting scholars, policy makers, practitioners, and advocates. Some of these events will be devoted to student presentations and discussions or debates, adding to the opportunities for building their skills as presenters and discussants.

4. Administrative and Disciplinary Identity of the Program. In keeping with its interdisciplinary mission, the doctoral program will not be housed within an existing academic department but instead will be located within the College of Basic and Applied Sciences.

5. Dissertation Topic and Advisory Committee Composition. In keeping with the interdisciplinary intent of the degree, the candidate's dissertation committee must include members representing at least two different disciplines (i.e., chemistry, biology, mathematics, etc.) and the majority of the program coordination committee must agree that the dissertation itself is interdisciplinary in scope.

J. Description of New Courses:

BIOL 6760 **Bioinformatics.** Four credits. Prerequisites: BIOL 1110 and 1120 and CSCI 1170 or consent of instructor. Explores the emerging field of bioinformatics which involves the application of computer science to biological questions. Specifically applies to the computational aspects of data gathering, processing, storage, analysis, and visualization methods for use in revising and testing biological hypotheses. Students should have a strong background in either computer science or biology, be willing to learn about the other field in an accelerated fashion, and be willing to work cooperatively as part of an interdisciplinary team.

BIOL 7400 **Computational Biology I**. Three credits. Emphasizes the fundamentals of evolution in virtual populations of digital organisms. The principles and methods used for modeling natural selection, genetic drift, mate-choice, and host-parasite co-evolution are covered.

BIOL7410 **Computational Biology II.** Three credits. Advanced topics and exposure to emerging research areas in the fields of computational biology are covered.

CHEM 7400 **Computational Chemistry I.** Three credits. Exploration of different molecular modeling techniques that can be used as adjunct to experimental research to provide new insights into chemical / biochemical problems. Topics covered: classical molecular modeling tools (molecular mechanics, molecular dynamics and Monte Carlo simulations); *ab-initio* quantum chemistry (SCF LCAO techniques, HF and post-HF methods); density functional theory and its applications; treatment of large systems (MM/QM and linear scaling QM methods); molecular similarity; elements of drug design. Intensive exploration of computer program packages: Sybyl, Spartan, Gaussian, ADF and Aimpack.

CHEM 7410 **Computational Chemistry II.** Three credits. Advanced topics in computational chemistry including an introduction to emerging research areas in computational chemistry are presented.

CSCI 6300 **Fundamentals of Programming Languages**. Three credits. Prerequisite: Sufficient background in algebra and trigonometry. Topics include basic high-level language constructs; data structures such as arrays, strings, records, stacks and queues, and linked lists; recursion, pointers, sorting and searching. Emphasis is on problem solving using the language and principles of structured software development.

CSCI 7200 **Scientific Programming.** Four credits. Basics of scientific computer programming. Emphasis is put on program design, algorithm development and verification. Students learn the basic usage of a chosen computing language, e.g., FORTRAN, C, or C++, and a chosen software tool, e.g., MATLAB. A variety of problems encountered in contemporary research in various scientific disciplines and solutions to these problems are discussed. Students are taught to develop algorithms for solving scientific problems and to implement the algorithms using the chosen programming language and software tool. No prior programming experience is required. Lecture and computer lab.

CSCI 7500 **Databases and Visualization.** Four credits. Topics include relational database design, relational algebra and query languages. Students are required to design a database for a chosen scientific application. Topics covered include principles of graph construction, the visual communication of data, and visualization methods. Includes rigorous, scientific discussion of graphical perception, the visual decoding of information from data displays. Software packages such as Data Visualization Toolbox for Matlab will be used.

CSCI 7350 **Data Mining** (**Selected Topics in Artificial Intelligence.)** Three credits. Prerequisites: CSCI 3110 and CSCI 5350. In-depth study of the principal areas of the field include artificial intelligence programming, problem-solving methods, knowledge representation methods, deduction and reasoning, and applications such as natural language processing and expert systems. May be repeated up to total of 6 hours if different topics.

COSC 6100 **Fundamentals of Computational Sciences**. Three credits. Pre requisite: Consent of advisor. Provides students with high-performance computational tools necessary to investigate problems arising in science and engineering, with an emphasis on combining them to accomplish more complex tasks. A combination of course work and lab work provides the proper blend of theory and practice with problems culled from the applied sciences. Includes review of mathematical tools for scientific applications and analysis.

COSC 7900 **Directed Research in Computational Science.** One to six credits. Designed for student research done in preparation for their doctoral project (before passing the qualifying exam). Involves the selection of a research problem in collaboration with a research mentor, review of pertinent literature, and determination and pursuit of a research strategy.

COSC 7950 **Research Seminar in Computational Science.** Two credits. Advanced reading, discussion, and presentations in computational science.

COSC 7640 **Dissertation Research.** 1 - 6 credits. Selection of a research problem, review of pertinent literature, and collection and analysis of data. Composition and formation of a dissertation committee is required. Once enrolled, student must register for at least one credit hour of doctoral research each semester until completion. S/U grading.

COSC 7800 **Teaching Internship.** Three credits. Students will teach a science course under the supervision of an experienced faculty mentor. Mentor will assist the student in preparing a syllabus, developing and teaching the class, and writing and administering assessment activities. The mentor will also provide the student with constructive feedback based on the student's teaching experiences.

MATH 6500 **Fundamentals of Scientific Computing.** Three credits. Introduction to numerical methods for students with diverse backgrounds in computationally-oriented disciplines who need to solve mathematical problems. Provides a comprehensive yet concise study of numerical methods for solving all the major problems in scientific computing, including linear and nonlinear equations, least squares, eigenvalues, optimization, interpolation, integration, ordinary and partial differential equations, fast Fourier transforms, and random number generators.

Students gain experience in using modern software packages and programming languages in scientific computing.

MATH 7100 **Applied Computational Science.** Four credits. Builds on *Fundamentals of Computational Science* and provides students with high-performance computational tools necessary to investigate problems arising in science and engineering, with an emphasis on combining them to accomplish more complex tasks. Topics include mesh generation, stochastic methods, basic parallel algorithms and programming, numerical optimization and nonlinear solvers. Example problems might be from Acoustics, bio-chemistry, or biological systems.

MATH 7300 **Numerical Methods**. Three credits. Prerequisites: Calculus I and II. Explores numerical analysis and its place in mathematics. Topics covered include: development of computer-friendly algorithms for solving transcendental equations and problems in Linear Algebra; numerical differentiation and integration with an emphasis on multi-variable functions; and approximate methods for initial-value and boundary-value problems for ODE, PDE and integral equations.

MATH 7400 **Computational Statistics.** Three credits. Prerequisite: Math 2050 or consent of instructor. Statistical visualization and other computationally-intensive methods of statistics. Emphasizes the role of computation as a fundamental tool of discovery in data analysis, of statistical inference, and for development of statistical theory and methods. Topics include Monte Carlo studies in statistics, computational inference, data partitioning and resampling, numerical methods in statistics, nonparametric probability density estimation, statistical models, and data fitting.

MATH 7450 **Mathematical Models in Biology.** Three credits. Explores use of models in biology in a wide range of topics, including ecological interactions, population biology, and evolutionary theory. Emphasis on the biological insights models can provide rather than mathematical techniques.

MATH 7750 **Mathematical Modeling**. Three credits. Prerequisites: Math 1920 or approval of instructor. Covers the principles of process and techniques for mathematical modeling. Emphasis is on deterministic and stochastic models. Main focus is on modeling dynamical systems using differential equations and difference equations. Other topics include optimization and evolution, stochastic processes and statistical methods, numerical simulation and applications in computational sciences and life sciences. Some acquaintance with basic differential equations and probability theory is desirable.

MATH 7800 **Parallel Computing.** Four credits**.** In-depth study of techniques for the design and analysis of parallel algorithms and for programming these algorithms on commercially available parallel platforms. Principles of distributed programming techniques, different parallel programming models with extensive coverage of MPI, POSIX threads, and OpenMP will be studied. Provides a broad and balanced coverage of various core topics such as sorting, graph algorithms, discrete optimization techniques, data-mining algorithms, and a number of algorithms used in numerical and scientific computing applications. Primary focus is to apply algorithms for efficient scientific computing on modern high-performance computers at Oak Ridge National laboratory.

PHYS 7400 **Computational Physics I.** Three credits. Students gain in-depth experience in adapting scientific problems from a variety of areas in physics into a form suitable for solution by numerical modeling methods. General objective of the course is to foster strong skills in expressing physical phenomena in mathematical form and then adapting these models for analysis using the techniques of computational physics. The primary tool to implement the techniques being taught will be MATLAB. Covers a number of the computational "standards" of modern physics such as chaotic dynamics, spectral analysis, Monte Carlo methods, and optimization techniques such as genetic algorithms and simulated annealing.

PHYS 7410 **Computational Physics II.** Three credits. Advanced topics in computational physics are covered including approaches to the solution of partial differential equation problems that arise in electrodynamics and the quantum mechanic description of matter.

FORMAT – PJ (Program Performance and Justification)

Institution: Middle Tennessee State University

Program Name: Ph.D. in Computational Science

Date: Fall 2009

A. **Accreditation**

There are no separate professional accrediting agencies for a Computational Science degree, but the departments of the college maintain affiliation or membership in the major professional associations of their disciplines. Middle Tennessee State University has been accredited by the Southern Association of Colleges and Schools (SACS) since 1962. The Office of Institutional Effectiveness, Planning, and Research coordinates planning and review for ongoing SACS accreditation and this doctoral program will be integrated into the current institutional effectiveness plan of the College of Basic and Applied Sciences.

Additionally, this degree program will be reviewed by an external reviewer on a regular five-year cycle in accordance with University, TBR, and THEC policy.

MTSU currently awards Doctor of Philosophy degrees and the development of this new degree has no implications for continuing SACS accreditation of the university.

B. **Evaluation Plans**

This Ph.D. program will provide for regular and systematic program evaluation. The assessment standards that are most appropriate for measuring the effectiveness and success of the proposed program are:

- congruence with and demonstrated achievement of the mission of the University set forth in the goals and objectives of the institutional effectiveness plan for the Ph.D. program and consistency with the university's Academic Master Plan;
- favorable external review;
- favorable exit interviews with students completing the Ph.D. program;
- favorable employment and career patterns for Ph.D. program students, including, but not limited to, publication of original scholarly work in the field; and
- how successfully students are able to meet the research objectives outlined in the graduation requirements, namely:
    - make at least two research presentations at regional, national or international meetings as the lead or co-author.
    - be lead author or make significant contribution as co-author of two articles published, in press, or under review in peer-reviewed journals.
    - make a significant contribution to the development of at least one external grant proposal.

The Office of Institutional Effectiveness is responsible for organizing and conducting official evaluations and programmatic reviews at MTSU related to the regular five-year external review mandated by TBR and THEC. Additionally, the College of Graduate Studies conducts a comprehensive review of every graduate program every five years. These reviews are conducted jointly and include development of a comprehensive self-study, student and alumni evaluations, employer data, and an on-site assessment of the program by a recognized expert serving as an external evaluator.

C. Evidence of Demand and Need

The Ph.D. degree in Computational Science has been developed because it offers an excellent match between the strengths of the University and the national need for enhanced computational science training with an interdisciplinary focus, as delineated in the report (described earlier in this document) *Computational Science: Ensuring America's Competitiveness* issued by the President's Information Technology Advisory Committee. Furthermore, the program is compatible with the wider call issued by the National Academy of Sciences for academic institutions to foster interdisciplinary research by changing degree programs, policies, and ideologies (*Interdisciplinary Research Urged, 2004, http://chronicle.com/prm/weekly/v51/i15/15a02502.htm*). Perhaps the best evidence for need is provided by the fact that a number of funding agencies are strongly encouraging the development of personnel in computational science. For example the Department of Energy (DOE) offers an extensive fellowship program described in *Building a Community of Leaders: The Department of Energy's Computational Science Graduate Fellowship* (*http://www.krellinst.org/csgf/commun_of_leaders/index.html*).
As explained in that report, the DOE Office of Science initiated the Fellowship program "because of the critical importance of computational science to their core missions, and a profound recognition of the nation's growing and continuing need for broadly trained advanced computational scientists in academia, industry and government laboratories." Clearly, this proposed degree, with its interdisciplinary emphasis addresses societal, labor market, and scientific need.

A 2005 report from the Council on Competitiveness entitled *High Performance Computing Users Conference: Supercharging U.S. Innovation & Competitiveness* (*http://www.compete.org/pdf/Conference_Report%20PR_01-10-2005.pdf*) stressed the importance of high performance computing and noted that one of the barriers to its effective application was the lack of personnel capable of using high-performance computing productively or of fully exploiting its potential for innovation. The Council conducted a survey which revealed that a shortage of qualified computational scientists was a significant impediment to broad commercial deployment of computational science tools, techniques, and infrastructure and that a similar concern was raised by researchers at national laboratories and universities. In terms of market size and growth potential, it is clear that continued progress in developing computing power will result in a concomitant need for those who can apply that power to solve complex applied problems.

Similarly, the report *Computational Science: Ensuring America's Competitiveness* issued by the President's Information Technology Advisory Committee in June 2005 (http://www.nitrd.gov/pitac/reports/20050609_computational/computational.pdf) outlines the vital importance for an emphasis on computational science saying that inadequacies in the national response "compromise U.S. scientific leadership, economic competitiveness, and national security" (p. 14). Significantly, this report recognizes that in order to properly prepare greater numbers of qualified individuals in computational science, a multidisciplinary approach of the type being proposed here is essential. The following quote is taken from the Principal Recommendation of that report:

> ***Universities and the Federal government's R&D agencies must make coordinated, fundamental, structural changes that affirm the integral role of computational science in addressing the 21st century's most important problems, which are predominantly multidisciplinary, multi-agency, multi-sector, and collaborative (p. 14).***

A key feature of the proposed Computational Science Ph.D. degree is that it prepares graduate students as computational scientists to solve problems in traditional disciplines; for example, biology, chemistry, physics, environmental sciences, and engineering. In terms of career opportunities, graduates would compete not only for jobs in colleges and universities but also for positions in business, industry, and at national labs that seek candidates with science-oriented computational skills. Examples from the business and industry category are manifest by the large number of computational scientists who have adapted their hard-science computational expertise into the fields of numerical biology (finding employment at medical research centers or in the biotechnology sector) and quantitative finance (finding employment at banks, hedge funds, and investment firms). At the national labs computational methods are a central element in both civilian applications such as materials science and engineering and for national security purposes, such as the use of supercomputer simulation to safeguard the nuclear stockpile necessary since the advent of the test ban treaty. This program is unique within Tennessee because it is focused on the use of computational methods to address fundamental problems in the areas of mathematical and scientific computing, including computational biology, data mining, medical data analysis, and materials science. The program will build on existing collaborations including those with Oak Ridge National Laboratory (MOU signed November 7, 2005) with their world-class computing facilities, and with Vanderbilt Ingram Cancer Center.

The graduates of the proposed Ph.D. in Computational Science will not only have the required academic and technical proficiency but will also be extremely adaptable, receptive, and responsive to the changing needs of the workforce. These graduates will be leaders of a diverse, globally-engaged, science and mathematics workforce required for the continued success of the State of Tennessee and of the United States.

The college-age population is expected to continue to grow through 2015, reaching an all-time high of 21.7 million. A well-prepared science and engineering (S&E) workforce is essential to the continued strength and growth of the U.S. economy. Census data indicates that the growth rate of the S&E job sector continues to grow at a rate that is triple that of the overall job market. The occupational projections based on Bureau of Labor Statistics (BLS) data are that S&E jobs will increase 70% faster than the overall occupation growth rate (*Science and Engineering Indicators 2006* *http://www.nsf.gov/statistics/seind06/pdf/c03.pdf*, Chapter 3 p. 8). Particularly germane for this proposal is that approximately 78% of BLS's projected increase in S&E jobs are in computer-related occupations. Personnel trained at the highest level in applied computation are, and will increasingly be, valuable members of the S&E workforce.

Educational Need: Traditional university curricula unavoidably limit students' ability to generalize information across discipline-specific courses. Students experiencing an interdisciplinary approach to problem solving, on the other hand, will develop skills and problem solving approaches applicable to many disciplines (see the report Graduate Education The Backbone of American Competitiveness and Innovation by the Council of Graduate Schools or the article *Practical aspects of practicing interdisciplinary science* **Computational Biology and Chemistry** Volume 27, Issue 3, July 2003, Pages 163-164). The proposed computational science program brings together students with computer expertise and students with a background in different disciplines of the natural sciences. It will challenge the former group with real-world scientific problems and provide the latter group with mathematical and computational tools as well as communication skills needed to solve these problems. The specific goals of the program are

- to offer broad and comprehensive training in computational methods in a manner that is not possible within traditional programs in individual departments,
- to emphasize an interdisciplinary, team-based approach to scientific problem solving,
- to help students develop superior communication skills needed to distribute results to the scientific and lay communities through publication and presentations, and a working knowledge of the process for acquiring external research funding,
- to recruit talented, independent-minded students with strong interests in natural sciences and computing,
- to foster critical, reflective, cross-disciplinary thinking by maintaining a culture of open dissemination of ideas in an environment where faculty and students are part of collaborative and interactive teams, and
- to train researchers and educators who are able to tackle a broad range of problems in a technology-driven research environment and who will thus be highly competitive in an ever-changing job market.

To accomplish these goals, students entering the Computational Science program with a bachelor's degree will complete 9 credits hours of foundational material, followed by a 36 credit hour core designed to give students a solid grounding in mathematical and programming skills necessary for research in Computational Science. Students entering with a master's degree may receive credit for up to 12 hours of coursework. Finally, students take 15 hours of elective coursework relevant to their areas of scientific specialization within computational science. Students will be participants in research groups performing directed research (6 hours in total before candidacy) from their first year on campus. After passing a qualifying exam, students will perform 12 hours of dissertation research culminating in a dissertation.

Student Interest/Demand: There is ample evidence of rising student demand for graduate programs in interdisciplinary science, and there are growing efforts to make students aware of opportunities in, and the importance of, computational science in particular. The 1999 edition of *Peterson's Guide to Graduate Study* introduced a new component called the Cross Disciplinary Announcement. The intent of this feature is to attract the interest of students from one disciplinary background either to look at opportunities in a different discipline or an emergent interdisciplinary field. Because the current and future generations of students are growing up in an environment where computers are ubiquitous, it is a natural fit for them to combine their interest in science with computation. Furthermore, there are a number of significant efforts to strengthen student interest in computational science by making younger students aware of the discipline and its opportunities and contributions to the progress of modern science. With support from the National Science Foundation, the National Computational Science Institute (NCSI) (*http://www.computationalscience.org*) created the Computational Science Education Reference Desk (CSERD) (*http://www.shodor.org/refdesk/*) as an informational tool for K-16 students and teachers. Other efforts include Carnegie Mellon University's creation, Alice (*http://www.alice.org/*), a free 3D interactive modeling environment used to introduce object-oriented programming to middle school, high school, and community college students and Little-Fe, a portable, educational eight node PC cluster (*http://contracosta.edu/hpc/resources/Little_Fe/*) used at schools and conferences to stir visible interest in Computational Science.

We conducted two assessments to verify a strong level of student interest in a Ph.D. in Computational Science. The first approach involved a local evaluation of the program's ability to recruit from MTSU students or from student contacts of MTSU Computational Science faculty. The second assessment estimated national interest in such a program by contacting other Computational Science graduate programs similar to the one we are proposing to ascertain their level of success at recruiting.

For the local estimate of student interest a simple needs assessment was done by canvassing the faculty members involved in the Computational Science Ph.D. program to ask them if they could locate students (with suitable qualifications) who would be interested in the program once it is started. We located over 10 students who expressed a serious interest in the program. This number of interested students was generated only through CS faculty contacts with previous MTSU students and via their interactions with students at other institutions. An electronic survey was also conducted to an additional 20 potential students to gain more in-depth information. Six individuals responded with three reporting a strong interest in the program, especially in the area of mathematical applications. Fifty percent of the overall respondents reported currently possessing a master's and one a doctorate. It is anticipated that we could generate much stronger numbers if the program were even modestly advertised regionally and nationally.

An electronic survey was also conducted to all of the graduating students from the College of Basic and Applied Sciences in Spring 2008. This survey garnered 99 replies of which 17 respondents said that they were "Definitely Interested" in the Computational

Science Ph.D. and 23 indicated that they “May be Interested.” This response was very encouraging given that it only targeted a small number of graduates from MTSU in a single semester. It is anticipated that we could generate much stronger numbers if the program were even modestly advertised regionally and nationally.

For a national estimate of the ability of our program to attract students, we contacted three programs that offered Computational Science Ph.D. programs and asked about their recruiting success. It is important to note that there are relatively few such programs—a majority of the programs that have a Computational Science emphasis (including most of those listed in Appendix A) award a Ph.D. in a traditional discipline area (e.g. Applied Math, Engineering) with the computational designation as an add-on to the conventional Ph.D. degree. We contacted 3 Computational Science Ph.D. programs at George Mason University, at Florida State University, and at San Diego State University. The results of our inquiries are summarized below.

George Mason University has a Computational Science Ph.D. program that is 17 years old and has 132 students enrolled. About 2/3 of their students are part time. They established an M.S. program in Computational Science about 5 years ago and they have about 12 students in that program—most students are more interested in the Ph.D. than the master’s.

San Diego State University offers a doctoral degree in computational science in conjunction with Claremont Graduate University. They currently have more than 40 students enrolled in the program and in a typical recruiting year they accept 15 students from a qualified pool of about 30 applicants.

Florida State University received approval for an M.S. program in Computational Science in Spring 2006 and approval for a Ph.D. in Fall 2007. They recruited 7 students into their initial master’s class of whom 5 are now in the Ph.D. program. In addition they recruited 13 students directly into the Ph.D. and another 3 will begin in the Spring bringing their total enrollment to over 20 in less than a year of existence. They report that they are recruiting nationwide with a high degree of student interest.

These analyses confirm that there is strong student interest in doctoral programs in computational science and we are confident given the contact base of our faculty and the experience and success of other programs that we can easily meet the recruiting goals we have set out.

Labor Market Evidence: Data published by the United States Department of Labor (2002) suggest that the employment projection (through 2012) for computer and applied mathematical occupations is much more favorable than for any other science profession (*www.bls.gov/news.release/ecopro.t02.htm*). The President’s Information Technology Advisory Committee Report on Computational Science (2005) notes that even with the emergence of computational science education programs over the past few years the number of graduates is inadequate to meet current demand and is far below the number that will be needed in the future. A white paper on high performance computing (HPC) prepared for the Council on Competitiveness revealed that this demand exists in academic institutions, national laboratories, and commercial settings (http://www.compete.org/pdf/HPC_Users_Survey.pdf). Indeed, a search conducted on the American Association for Advancement in Science (AAAS) job site in December 2006 yielded 49 jobs for computational scientists (34 academic jobs, 15 industrial or national labs) and 15 computationally oriented post-doctoral positions. Employment listings in major scientific journals or computer bulletin boards (*http://recruit.sciencemag.org*, *http://www.nature.com/naturejobs/*, *http://net.bio.net/hypermail/biojobs/*, *http://www.genomeWeb.com/careers/jobs.asp*) illustrate the high and growing demand for skilled computational scientists.

Industrial companies and governmental research organizations look for professionals with an ever-broader scientific background and range of skills, including not only technical knowledge but also communication and other interpersonal skills. Characteristic of current trends in the science job market is an increasing need for three types of specialists (*www.bio-itworld.com/careers/mapping/1468.html*) :

a.) experts who, in addition to an extensive background in basic sciences, have an understanding of the strengths and limitations of computational analysis,

b.) method developers who can efficiently find new approaches to analyzing data, and

c.) software engineers who are able to produce robust tools for database design and data mining.

D. Human Resource Needs

1. *Faculty*:

Existing faculty will be able to absorb the teaching and advisement responsibilities during the start up years (1-3) because MTSU already has strong existing programs in Mathematics, Biology, Physics, and Chemistry. As enrollments grow and student involvement in courses and dissertation research increases, it is reasonable to expect that one additional faculty member will be added in year three. This position and any additional faculty will be supported by increased enrollment.

2. *Administrative*:

One individual will serve as the coordinator for the program. This Computational Science Graduate Coordinator will receive six (6) credits reassigned time each semester during the academic year and a summer stipend. We anticipate that this position will be filled by an existing faculty in the College of Basic and Applied Sciences who will also teach courses and advise students in the proposed program. The department in which this person is tenured will be provided adjunct replacement for the proportionate reduction of teaching service to the department.

3. *Support Staff*:

A computer support technician will be required to help with the configuration and maintenance of computing and network facilities.

Postdoctoral research associates are common in science Ph.D. programs across the country and form an integral part of any science Ph.D. program because they provide an extra resource for graduate student success. Once the Ph.D. program is established, postdoctoral scholars will be funded through grants.

E. <u>Other Needs for Support</u>

1. *Library*:

Because the university already has graduate programs in the departments supporting this proposed degree, significant library holdings are already in place. However, to assure the highest level of research support for the program, we plan to enhance library holdings and subscriptions. We plan an initial investment of $5,000 per year in years one through three. An additional infusion of $10,000 recurring annual expenditure is anticipated for journal subscriptions and access fees for electronic databases beginning in year one.

2. *Instructional Facilities:*

If approved, the program will start in Fall 2009. A new 258,000 ft^2 Sciences Building will be completed in 2011. Many of the computational science faculty and some of the computational equipment will be housed in this new state-of-the-art facility. In addition, classroom and research space will be available for use by the faculty and students involved in the proposed computational science Ph.D. program.

3. *Instructional and Research Equipment*:

Over the last two years, MTSU has invested nearly $94,000 in new computational facilities and equipment for use by faculty in Computational Science. This equipment includes a Beowulf-type high-performance Linux computing cluster consisting of one 8-processor server and nine 8-processor production nodes (total 80 processors) connected together via a gigabit network. The cluster has an aggregate of 164 gigabytes of memory and over 9 terabytes of disk space. Going forward, computer workstations will be needed for each full-time graduate assistant ($1,200 per computer).

4. *Other Needs*:

Assistantships ($18,000 per student per year) will be the principal means by which the program will support students. Assistantships also represent strong incentives for recruitment of out-of-state students to the program.

Recruitment will also involve expenditures. Costs associated with these efforts include printing of brochures, announcements in professional journals, travel to conferences, display boards for use at conferences, printing announcements and related materials included in informational packets for mailing to deans and department chairs at various colleges/universities around the country, descriptive materials and applications for potential applicants. Office resources will also be needed. This will include expenses associated with telephone, stationery, and postage.

Student and advisor travel to present research findings at professional conferences will receive some support within the program. Student participation at such conferences will bring visibility to the program (for purposes of recruitment) and to the quality of our degree candidates as they begin to seek post-degree employment.

F. Program Duplication

A recent national survey (*http://www.krellinst.org/learningcenter/CSE_survey/*) lists more than 30 M.S. and/or Ph.D. programs in computational science (see Appendix 3), but most of these are offered within a home science department (discipline specific degrees, such as computational biology, computational chemistry, computer science and applied mathematics) and only 15 are truly interdisciplinary in the sense that is being proposed here. Even fewer have a major specifically in computational science.

A Ph.D. in Computational Engineering exists at the University of Tennessee at Chattanooga. This proposed Ph.D. complements rather than competes with this existing program in that it resides exclusively in the natural sciences and mathematics and no engineering department is involved. The University of Tennessee offers a Ph.D. in computer science with a concentration in computational science but does not offer a major in computational science. Additionally, two highly specialized programs exist at the University of Memphis (master's in computational physics and Ph.D. computational chemistry), but these concentrations are narrowly focused on problems within a single discipline.

FORMAT SE (Student Enrollment Projections)

Estimate the headcount and full-time equated enrollment and the number of graduates for a complete program cycle.

Year	Full-Time[1] Headcount	Part-time[2] Headcount	Total Year Headcount	FTE	Graduates[3]
1	5	0	5	5	0
2	10	0	10	10	0
3	14	0	14	14	0
4	18	0	18	18	2
5	20	0	20	20	4

FTE is calculated based upon the following assumptions:

1 Full-time students are enrolled in 9 or more hours.
2 No part-time students will be admitted.
3 The expected time to graduation from the bachelor's level is between 5 and 6 years.

THEC Financial Estimate Form
Middle Tennessee State University
Ph.D. in Computational Science

Five-year projections are required for baccalaureate and post-baccalaureate programs and certificates. Three-year projections are required for associate degrees and undergraduate certificates. Projections should include cost of living increases per year.

	Year 1	Year 2	Year 3	Year 4	Year 5
I. Expenditures					
A. One-time Expenditures					
New/Renovated Space	$ -	$ -	$ -	$ -	$ -
Equipment	17,000	-	-	-	-
Library	5,000	5,000	5,000	-	-
Consultants	-	-	-	-	-
Travel	-	-	-	-	-
Other	-	-	10,000		-
Sub-Total One-time	$ 22,000	$ 5,000	$ 15,000	$ -	$ -
B. Recurring Expenditures					
Personnel					
Administration					
Salary	$ 14,400	$ 14,400	$ 14,400	$ 14,400	$ 14,400
Benefits	1,200	1,200	1,200	1,200	1,200
Sub-Total Administration	15,600	15,600	15,600	15,600	15,600
Faculty					
Salary	$ -	$ -	$ 60,000	$ 63,000	$ 66,150
Benefits	-	-	21,000	22,050	23,153
Sub-Total Faculty	$ -	$ -	$ 81,000	$ 85,050	$ 89,303
Support Staff					
Salary	$ 33,000	$ 34,650	36,383	38,202	40,112
Benefits	11,550	12,128	12,734	13,371	14,039
Sub-Total Support Staff	$ 44,550	$ 46,778	$ 49,116	$ 51,572	$ 54,151
Graduate Assistants					
Salary	$ 90,000	$ 180,000	$ 252,000	$ 324,000	$ 360,000
Benefits	-	-	-	-	-
Tuition and Fees* (See Below)	42,810	89,901	132,154	178,409	208,143
Sub-Total Graduate Assistants	$ 132,810	$ 269,901	$ 384,154	$ 502,409	$ 568,143
Operating					
Travel	$ 20,000	$ 20,000	$ 20,000	$ 20,000	$ 20,000
Printing	-	-	-	-	-
Equipment	6,000	6,000	4,800	4,800	2,400
Other	10,000	10,000	10,000	10,000	10,000
Sub-Total Operating	$ 36,000	$ 36,000	$ 34,800	$ 34,800	$ 32,400
Total Recurring	$ 228,960	$ 368,279	$ 564,671	$ 689,431	$ 759,597
TOTAL EXPENDITURES (A+B)	**$ 250,960**	**$ 373,279**	**$ 579,671**	**$ 689,431**	**$ 759,597**

*If tuition and fees for Graduate Assistants are included, please provide the following information.

	Year 1	Year 2	Year 3	Year 4	Year 5
Base Tuition and Fees Rate	$ 8,562.00	$ 8,990.10	$ 9,439.61	$ 9,911.59	$ 10,407.16
Number of Graduate Assistants	5	10	14	18	20

II. Revenue

	Year 1	Year 2	Year 3	Year 4	Year 5
Tuition and Fees[1]	42,810	89,901	132,154	178,409	208,143
Institutional Reallocations[2]	208,150	283,378	447,517	511,022	551,454
Federal Grants[3]	-	-	-	-	-
Private Grants or Gifts[4]	-	-	-	-	-
Other[5]	-	-	-	-	-
TOTAL REVENUES	**$ 250,960**	**$ 373,279**	**$ 579,671**	**$ 689,431**	**$ 759,597**

Notes:

1. In what year is tuition and fee revenue expected to be generated and explain any differential fees. Tuition and fees include maintenance fees, out-of-state tuition, and any applicable earmarked fees for the program.

   Tutition and Fees are calculated conservatively, using projected 2008 in-state tuition rates and factoring a 5 % annual tuition rate increase.

2. Please identify the source(s) of the institutional reallocations, and grant matching requirements if applicable.

   The amount is derived from reallocation of existing resources including technology access fees and indirect costs collected on grants and contracts. As external funding is obtained, institutional support will be reduces accordingly.

3. Please provide the source(s) of the Federal Grant including the granting department and CFDA number.

4. Please provide the name of the organization(s) or individual(s) providing grant(s) or gift(s).

5. Please provide information regarding other sources of the funding.

NOTES FOR EXPENSES:

Graduate Coordinator has six credit hours reassigned each semester, in addition to a $6,000 stipend in the summer.

Travel costs are included to provide for faculty, student, and visiting speakers' travel in in support of the program.

Other expenses include funds for purchase of computers and related equipment and $10,000 per year for print and online journal subscriptions and database subscriptions.

Appendices

1. Suggested Schedule of Study
2. Dissertation Topic and Committee Composition
3. Survey of Computational Graduate Programs
4. Architect's Drawings of MTSU Sciences Building
5. Summary of Faculty Experience and Expertise
6. Faculty Vita**e**

Appendix 1. Suggested Schedule of Study.

The following schedule is an example of a schedule typical for a student entering with a bachelors degree.

Year 1 – Fall semester	COSC6100	Fundamentals of Computational Science	3
	MATH6500	Fundamentals of Scientific Computing	3
	CSCI6300	Fundamentals of Programming Languages	3
	MATH7300	Numerical Methods	3
	COSC7950	Comp. Sci. Research Seminar	2
Year 1 – Spring semester	CSCI7500	Databases and Visualization	4
	CSCI7200	Scientific Programming	4
	MATH7400	Computational Statistics	3
	COSC7800	Teaching Internship	3
	COSC7950	Comp. Sci. Research Seminar	2
Year 1 – Summer semester	COSC7900	Directed Research Computational Science	3

NOTE: At the end of the Spring semester of Year 1, the student will decide on composition of dissertation committee and dissertation topic (see next section).

Year 2 – Fall semester	MATH7800	Parallel Computing	4
	MATH7100	Applied Computational Science	4
	MATH7750	Mathematical Modeling	4
		Elective #1	3
Year 2 – Spring semester		Elective #2	3
		Elective #3	3
		Elective #4	3
Year 2 – Summer semester	COSC7900	Directed Research Computational Science	3

NOTE: At the end of the 2nd year in the program, the student will take preliminary exam (see below).

Year 3 – Fall semester		Elective #5	3
	COSC7640	Dissertation Research	3
Year 3 – Spring semester	COSC7640	Dissertation Research	3-6
Year 3 – Summer semester	COSC7640	Dissertation Research	3-6
Year 4 – Fall semester	COSC7640	Dissertation Research	3-6

Year 4 – Spring semester	Dissertation Research	3-6
Year 4 – Summer semester	Dissertation Research	3-6
Year 5 – Fall semester	Dissertation Research	3-6
Year 5 – Spring semester	Dissertation Research	3-6

NOTE: At the end of the Spring semester of Year 5 (if not earlier), the student will defend dissertation (see next section).

The preliminary exam will consist of a written portion and an oral portion. The composition of each portion will be reflective of the student's prior coursework and chosen area of research, and will be decided upon by the student's dissertation committee (see next section) by the end of the Fall semester of Year 2. Students will be given two attempts to pass the preliminary exam; the second attempt must occur not later than the end of the Fall semester of Year 3. Students who do not pass on the second attempt will be allowed to continue in the program through the end of the Spring semester of Year 3. At that point, a student who has failed both attempts of the preliminary exam will be given the option of enrolling into the master's program in the Department of Mathematics, Chemistry, Biology, or Computer Science. Relevant coursework taken toward the Ph.D. in Computational Science will be transferred and substituted with permission of the department chair. If a student is admitted into the master's program in a department, the student must satisfy all of the requirements of that degree to be awarded a master's degree.

Appendix 2. Dissertation Topic and Committee Composition:

The dissertation topic will be decided between the student and the major professor but with input and oversight from the student's dissertation committee. Each committee member must be a full member of the Graduate Faculty, and the Chair of the Committee must be a doctoral-level graduate faculty member. The dissertation committee will be composed of 5 members including the major professor. If the student and the dissertation chair feel that an external committee member from either a department not participating in the Computational Science Ph.D. program, another university, or a government laboratory (such as Oak Ridge National Laboratory) can provide additional expertise vital to the research direction, then this person can serve as a committee member after obtaining adjunct graduate faculty status from the Graduate Council.

The committee will be charged with

- monitoring the quality of scholarship of the research, ensuring that it addresses a problem of sufficient interest that its solution would warrant publication in the scientific literature, and
- ensuring a particular emphasis on problems that cross disciplinary lines or that synthesize methods or concepts from two or more disciplines by having representation by at least one member from a second discipline that is most related to the research problem and a member whose research interests and specialization do not directly relate to the dissertation topic.

Once formed, the student and the committee will meet to finalize the topic of the dissertation. The dissertation topic will be presented to the committee in the form of a written proposal (4-8 pages), and must be approved by the dissertation committee and the Program Coordination Committee (see section I below).

The student and the committee will meet formally once per semester during the academic year to review progress in coursework and research. The committee will make recommendations in both areas and will ensure that the student's research maintains an interdisciplinary focus.

The committee will design and administer the preliminary exam, with successful completion of this exam requiring a simple majority vote of the committee. Successful defense of the dissertation will require the approval of all committee members.

Appendix 3 –Computational Science & Engineering Programs in U.S.

Baylor College of Medicine	PhD in Structural & Computational Biology & Molecular Biophysics
Boston University	CSE courses through the Center for Computational Sciences
California Institute of Technology	PhD in Applied & Computational Mathematics with several concentrations
Carnegie-Mellon University	Minors in science departments
Clemson University	CSE courses in the Computer Science Department
Colorado State University	MS in Applied and Computational Mathematics
Cornell University	CSE courses; PhD in Applied Mathematics includes Computational Science
Duke University	CSE certificate, Center for Computational Science and Engineering
Florida State University	PhD from home department; CSE department degrees
George Mason University	PhD in Computational Sciences and Informatics
George Washington University	CSE Courses in the Physics Department
Indiana University at Bloomington	PhD Minor in Scientific Computing
Louisiana Technical University	PhD in Computational Analysis and Modeling
Louisiana State University	Dual Physics PhD/Computer Science MS
Massachusetts Institute of Technology	CSE courses in Mathematics and EE & Computer Science Departments
Mississippi State University	MS, PhD in Computational Engineering
New York University, Courant Institute	MS in Scientific Computing
North Carolina State University	Specialty degree as an extended minor
The Ohio State University	CSE courses in Computer and Information Science Department
Princeton University	PhD, Program in Applied and Computational Mathematics
Purdue University	MS, PhD in traditional department with a specialization in CSE
Rensselaer Polytechnic Institute	MS, PhD from home department with CSE certificate
Rice University	Professional Master's degree, PhD in CSE
San Diego State University	MS, PhD in Computational Science

Stanford University	MS, PhD, Scientific Computing and Computational Mathematics
Syracuse University	CSE programs through the Northeast Parallel Architectures Center
University of Arizona	PhD minor in CSE
University of California at Davis	Ph.D. in Applied Science with Emphasis in Computational Science
University of California at San Diego	PhD, Program in Scientific Computation (planned)
University of Colorado	CSE courses in Department of Computer Science
University of Illinois, Chicago	PhD and MS in Computational Science and Applied Mathematics
University of Illinois, Urbana-Champaign	MS, PhD in traditional department with a specialization in CSE
University of Iowa	Interdisciplinary PhD, Department of Applied Mathematics and Computer Science
University of Louisiana, Lafayette	MS, PhD in Computational Science and in Computational Engineering
University of Michigan	PhD in discipline with "..and Scientific Computing"; MS in Scientific Computing
University of Minnesota	MS, PhD in Scientific Computing
University of Nevada, Las Vegas	CSE courses, Mathematical Sciences Department
University of New Mexico	MS, PhD in home department with a certificate in CSE
University of North Carolina, Chapel Hill	Interdisciplinary programs
University of Oregon	Interdisciplinary Computational Science Institute
University of Pittsburgh	PhD in Computational Biology
University of San Francisco	Computational science thesis for MS
University of Texas at Austin	MS, PhD in Computational and Applied Mathematics
University of Utah	MS and graduate certificate in Computational Engineering and Science
University of Wisconsin	Professional Master's Degree Program in Computational Sciences
Vanderbilt University	CSE courses in Physics & Astronomy and Computer Science Departments

Appendix 4.

Architect’s Drawings

Sciences Building

Middle Tennessee State University

Appendix 5 Summary of Faculty Experience and Expertise

The following table summarizes the extent of experience with Ph.D. thesis supervision, research, publication, and other doctoral level experience within the Computational Science Faculty. Full details of the faculty members' experience is given in the faculty vitae provided in Appendix 6.

Faculty	Highest Degree	Institution	Masters students	Ph.D. students	Other doctoral experience	Refereed publications
Don Hong	Ph.D.	Texas A&M	14			44
Tibor Koritsanszky	Ph.D.	Free University of Berlin	3	6		116
Yuri Melnikov	Ph.D.	Dnipropetrovsk National State Univ.		11	4 D.Sc. candidates	25
Rong Luo	Ph.D.	West Virginia University				22
Cen Li	Ph.D.	Vanderbilt Univ.	8			9
Xiaoya Zha	Ph.D.	Ohio State Univ.				36
Stephen Howard	Ph.D.	Indiana Univ.				8
Abdul Khaliq	Ph.D.	Brunel Univ.	10		External examiner for 4 Ph.D. theses	52
William Robertson	Ph.D.	Purdue Univ.			External examiner for 2 Ph.D. theses	44
Anatoliy Volkov	Ph.D.	SUNY Buffalo				29

Appendix 6

Faculty Vitae