

# **INNOVATIVE GRADUATE PROGRAM IN COMPUTATIONAL SCIENCE AND ENGINEERING**

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**Computational Science and Engineering Program  
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North Carolina Agricultural and Technical State University (NCA&T) has established a master's degree program in Computational Science and Engineering (CSE). The program will be highly interdisciplinary, drawing expertise and resources from various disciplines across the University, and operating outside a department. It will offer an interdisciplinary curriculum combining applied mathematics, high performance parallel and scalable computing, scientific modeling and simulation, data visualization, and domain areas such as physical science and engineering, life sciences, agricultural and environmental sciences, technology and business. The aim of this program is to provide students with an opportunity to (a) master high performance computer programming tools as well as data acquisition and processing techniques; (b) acquire computational modeling, simulation and visualization skills; (c) relate acquired computational science and engineering knowledge and skills to specific application fields of science, engineering, technology and business; and (d) learn to develop novel and robust computational tools and methods to solve scientific, engineering, technological or business problems. Graduates of this program will be highly versatile computational scientists, engineers, technologists or business executives with a good understanding of the connections among various disciplines, and capable of interacting and collaborating effectively with scientists, engineers and other professionals in other fields.

The newly established MS degree program in CSE builds upon the University's curricular strength and research capability in science, engineering, mathematics, technology, and business. It is a result of interdisciplinary collaboration among the College of Arts and Sciences, College of Engineering, School of Agriculture and Environmental Sciences, School of Business and Economics, and the School of Technology. It will enhance and supplement current graduate research and education programs in science, engineering, mathematics, technology and business, and further the fertilizing and nurturing of cross-disciplinary interaction and collaboration in CSE among faculty and graduate students. As the first stand-alone CSE graduate degree program in the State of North Carolina and among HBCUs in the nation, the program will increase the eminence of North Carolina A&T State University in this keen technological area.

The graduate degree program in computational science and engineering is an inter-disciplinary Master of Science program, involving the College of Arts and Sciences, College of Engineering, School of Agriculture and Environmental Sciences, School of Business and Economics, and the School of Technology. This CSE master's program would have three tracks with a focus on computational science, but distinguish across the domain areas of specialization. The three tracks with a common curriculum in their core courses will account for the variations in computational science field requirements across the several domains. The tracks are interdisciplinary in nature, and are primarily based on the variations in the background and training in the computational areas between the undergraduate domains. These are not grouped to conform to the individual colleges/schools these domain areas come under.

### Computational Science and Engineering

This track is designed primarily for students with undergraduate degrees in engineering, physics, mathematics, and computer science who will be trained to develop problem-solving methodologies and computational tools as well as interdisciplinary technical expertise in CSE for solving challenging problems in physical science, engineering, applied mathematics or computer science. This includes domains that are both in the College of Engineering, and the College of Arts and Sciences. The curriculum will emphasize computational sciences and engineering along with training in the domain areas. The goal of this track is to produce scientists, and engineers with focus, training and application in computational sciences, scalable computing, physics-based modeling and simulations, and with expertise in the application of computational techniques and principles in their primary domain areas. Qualified undergraduate students can be admitted to this stream if they also meet the admission criteria of their major domain field. Based on their undergraduate degrees, the students in this track would be required to have had an increased level of prior training, courses and exposure to mathematics including areas such as numerical analysis and to a high level programming languages. Students with undergraduate degrees in other science and technology areas may also be admitted, if they meet the admission and course requirements, including pre-requisites of the domain department. The areas of specialization will include, but will not be limited to, computational quantum chemistry, computational nuclear and high energy physics, computational solid or fluid dynamics, computational material science, bioengineering, engineering design and automation, applied and environmental geophysics, computational seismology, nonlinear computational mechanics, super fast algorithms for numerical and algebraic computation, and distributed and high performance computing.

### Computational Sciences

This track is designed primarily for students with undergraduate degrees in chemistry, biology, business, and agricultural sciences who will be trained to apply or extend computational tools and methods as well as data acquisition, processing and visualization techniques to study

computationally intensive problems in life sciences, agricultural and environmental sciences, and business and economics. This track primarily includes domain areas with lesser training in mathematics including numerical analysis, programming languages and focuses on domains with non-deterministic models. The domains in this track are from the College of Arts and Sciences, the School of Agriculture and Environmental Sciences, and the School of Business and Economics. The goal of this track is to produce biological and life scientists, business professionals and economists, and agricultural scientists with focus and expertise in computational sciences and the primary domain areas. Qualified undergraduate students can be admitted to this stream if they also meet the admission criteria of the major domain area. Based on their undergraduate field, the students in this track would be required to take additional mathematics and programming focused courses. Students with undergraduate degrees in other science, engineering and technology areas may also be admitted if they meet the admission and course requirements, including pre-requisites for the domain department. The areas of specialization will include, but will not be limited to, bioinformatics, computational genomics, computational physical chemistry, computational biochemistry, and computational finance.

### Computational Technology

This track is designed primarily for students with undergraduate degrees in technology disciplines with focus on computational science and engineering. These technology disciplines currently include computation technology, computer numerical control machining, remote sensing, GIS/GPS data analysis, and nanotechnology with additional potential disciplines in the future. The goal of this track is to produce technologists with a focus and training in computational sciences, and in their primary technology domain area. Students with undergraduate degrees in engineering, mathematics, physics and computer science may also be admitted and must meet the course and curriculum requirements in technology.

### Educational Objectives of the Program

The educational objectives of the program are as follows:

- Educate and graduate students with a mastery of high performance computer programming tools as well as processing, data acquisition, analysis techniques.
- Acquire, educate and train in computational modeling, simulation and visualization.
- Relate acquired computational science and engineering knowledge and skills to specific application fields of engineering, science, technology and business.
- Learn to develop novel and robust computational methods and tools to solve scientific, engineering, and technological and business problems.
- Produce highly versatile computational scientists, engineers, technologists, or business executives with a good understanding of the connections among various disciplines and capable of interacting and collaborating effectively with scientists, engineers, and professional in other fields.

- Increase the number of graduate professionals available to work in computational science and engineering.
- Increase the diversity of graduate professional especially underrepresented minority and African Americans available to work in computational science and engineering area.
- Assist the State of North Carolina and the nation to increase the pool of graduates with training and experience in computational science and engineering, interdisciplinary applications and research.

### Relationship to Other Programs

Several academic disciplines are related to the interdisciplinary graduate M.S. program in computational science and engineering. CSE is an interdisciplinary program drawing courses, research, faculty and students from two colleges - Arts and Sciences, and Engineering, and three schools - Agriculture and Environmental Sciences, Business and Economics, and Technology. The program will be supported by the current and emerging strengths in the computational areas of science, engineering, and technology, including infrastructure developments in high performance, scalable computing, and large-scale modeling and simulations. Several faculty and funded research projects exist in the areas of computational sciences and engineering. These will provide the research expertise and infrastructure that enhance the computational science and engineering programs. Computational techniques have already become an integral part of scientific discovery processing and engineering design in addition to experimental and analytical techniques. The demand for computational scientists, engineers and technologists in several critical areas of national interest is continually increasing. The graduate master's program will help meet the increased human resource needs in several areas of computational sciences, engineering and technology. The program will capitalize on the existing and emerging research strengths in computational science and engineering; and dovetail the FUTURES initiative with a focus on computational science and engineering to increase the eminence of North Carolina A&T State University in this keen technological area. Additionally, the program will educate, train and graduate under-represented professionals in computational science and engineering, especially African Americans.

### Courses

Courses for the CSE degree program will build upon courses in existing master's degree programs in the sciences, engineering, mathematics, technology, and business, yet will address the goals and objectives of the CSE program. Many of the disciplines and degree programs on campus have in place courses that support the CSE master's degree. For example, numerical linear algebra, numerical PDEs, scientific visualization, distributed and high performance parallel computing, computer organization and scientific programming, data structure, software tools, and computational science and engineering courses already exist in applied mathematics, computer science, physics, biology and mechanical engineering master's programs. Selected existing courses will be used or modified as core courses and others as interdisciplinary or domain elective courses for the program. A few new courses including several core courses for

computational sciences and computational technology as well as a couple of bridge courses will be developed for the program.

### Faculty

The CSE affiliated faculty of North Carolina Agricultural and Technical State University are active professionally, respected, and talented. Many have published research in respected journals or referred conference proceedings and have ongoing sponsored research projects in the areas of computational sciences and engineering. All faculty involved in the CSE master's program have strong records in research, publications and student research supervision. The Colleges of Arts and Sciences and Engineering have already hired three CSE faculty in mathematics, computer science and mechanical engineering, and the departments of mathematics and chemistry have recently advertised to fill up two positions in computational biomathematics and computational chemistry, respectively. Additionally, through enrollment growth funding the University will commit to the strategic hiring of additional new CSE faculty to strengthen this program. Considering the current faculty, and the anticipated infusion of new faculty with appropriate expertise in computational science and engineering, NC A&T has the necessary faculty expertise and intellectual underpinnings for a respected interdisciplinary CSE master's program.

### Societal Needs

The computational science and engineering program is a rapidly growing interdisciplinary endeavor with connections to the sciences, engineering, technology, mathematics and computer science. CSE involves the use of computational architecture to develop numerical algorithms or methods to study scientific or engineering problems.

CSE has emerged as a powerful and indispensable method to analyze a variety of problems in research, production and process development, and manufacturing. Computational modeling and simulation is being accepted as a third methodology in scientific discovery processing and engineering design, complementing the traditional approaches of theory and experiment. Many experiments and investigations that have traditionally been performed in a laboratory or the field are being augmented or replaced by computational modeling and simulation. Examples include weather and climate modeling <sup>1</sup>, fossil fuel combustion simulation <sup>2</sup>, engine and vehicle design <sup>3</sup>, materials development <sup>4</sup>, aircraft design <sup>5</sup>, electronic design automation <sup>5</sup>, and drug design and development <sup>6</sup>. Scientific visualization is another primary element of CSE, and has become an essential tool for the preprocessing of data sets and the investigation of massive amounts of computational results, as increasingly evident in bioinformatics, finance, and the mining of huge data sets <sup>7</sup>. Computational modeling, simulation, and visualization are immensely useful for studying things that are otherwise too big, too small, too expensive, too scarce, or too inaccessible to study.

Even though CSE makes use of the techniques of applied mathematics and computer science for the development of numerical algorithms and computing tools to the study of scientific and engineering problems, it is by no means a subfield or extension of applied mathematics or computer science, nor is it a discipline where a scientist or engineer simply uses a canned code to simulate data and visualize results. "CSE is a legitimate and important academic enterprise," as noted in a comprehensive, report <sup>5</sup> published by the SIAM Workgroup on CSE on Graduate Education in CSE. "Although it includes elements from computer science, applied mathematics, engineering and science, CSE focuses on the integration of knowledge and methodologies from all these disciplines, and as such is a subject which is distinct from any of them." The following figure, which has been widely accepted in the CSE community, reflects the view that besides connecting the sciences, engineering, mathematics, and computer science, CSE also has its own

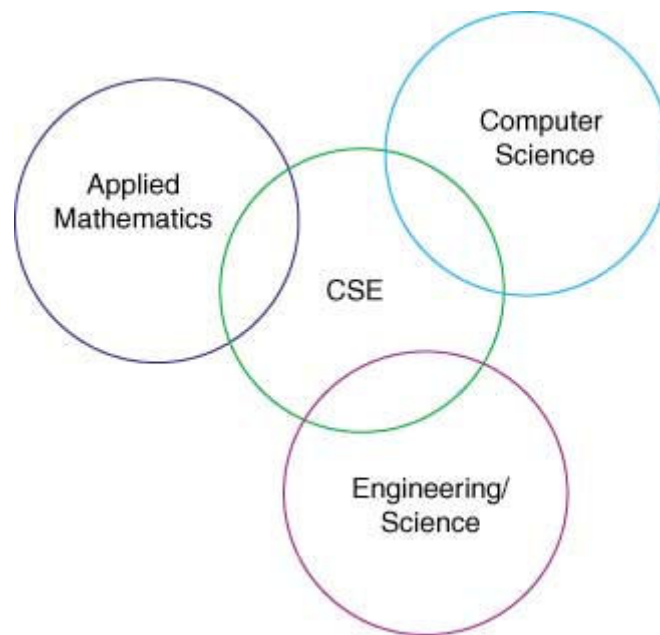


Figure 1: Interdisciplinary Nature of the CSE Program

core of elements that draws together and bridges all these disciplines. Such a CSE core is made up of a collection of computationally intensive problem-solving methodologies and robust tools, which constitute the building blocks for the study of scientific and engineering problems of ever increasing complexity and realism.

As suggested by Yasar and Landau <sup>8</sup>, CSE education has been evolving in three stages. The first stage, dating back to the 1980's and infused by the 1982 Lax report <sup>9</sup>, was recognition of the paradigm shift in which computation was accepted as a third methodology, joining theory and experiment as the basic techniques of scientific research and engineering design. The second stage of CSE occurred in the 1990's and marked its infancy <sup>10-12</sup>. During this period of time, a

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few CSE courses or experimenting curricula, primarily at doctoral level, started to be offered by those who were familiar with CSE ideas from their research and recognized the importance of integrating CSE research into education to meet the demand of computational professionals in this emerging interdisciplinary area. Commencement of the DOE Computational Science Graduate Fellowship Program <sup>13</sup> and issuance of the President's Information Technology Advisory Committee Report <sup>14</sup> were two of the milestones in this stage. The third stage, which began in 2000 and is expected to extend to 2010, is considered as early growth <sup>15-16</sup>. This current and ongoing stage is going to be characterized by a number of CSE courses and curricula being designed and implemented by various institutions at baccalaureate, master's and doctoral levels.

The 2001 SIAM report <sup>5</sup> and a recent Krell Institute report <sup>17</sup> by Swanson in November 2003 entailed the progress in CSE program development. However, the majority of these programs were established by major research universities, either at doctoral level or affiliated with doctoral programs. Even though there are a few smaller universities or liberal arts colleges that made the Krell Institute list, their programs are primarily at undergraduate level, and are mostly offered as a minor or concentration in computational science. Furthermore, no single HBCU (Historically Black College and University) makes either list. To meet the demand for computational science and engineering professionals, it is imperative that the participation of master's-focused institutions and HBCUs in computational science and engineering workforce preparation be included. HBCUs will prove essential in graduating minority students to help fill the gap in the area of CSE, and North Carolina Agricultural and Technical State University, a leading producer of minority baccalaureate degrees in sciences, mathematics, engineering, and technology programs in the nation, is well positioned to assist in addressing this concern.

Information and computational technology has been recognized as one of the engines of economic growth during the last decade, as evident by the President's Information Technology Advisory Committee's (PITAC) report <sup>14</sup>. The PITAC predicated a need of approximately one million people in information and computational technology, a need that cannot be met solely by current academic programs in science, technology, engineering and mathematics (STEM). The National Science and Technology Council have repeatedly reported the concerns of industry and national laboratories that the growing needs for well-trained computational scientists, engineers and technologies are not being satisfactorily met. We have seen that this nation has relied overly on people trained in information and computational technology from foreign countries. In addition, government initiatives such as the Presidential Information Technology Initiative, NSF's Information Technology Research (ITR) and Computational Neuroscience programs, and the DOE's Advanced Simulation and Computing (ASCI) and Scientific Discovery through Advanced Computing (SciDAC), and NIH's National Centers for Biomedical Computing and Centers for Bioinformatics and Computational Biology programs rely on people with scientific as well as computing knowledge and expertise. The demand for well trained computational scientists, engineers and technologies is significant.

The rapid growth of information and computational technology and its applications in the job market has created a need for multi-skilled workers at all levels, including the master's. The obvious preference of many employers to hire people with education in multiple disciplines suggests that having multiple skills and majors improve one's marketability and employment survival time. However, attaining multiple degrees is both costly and time-consuming. As an

alternative, an interdisciplinary CSE education program can save time and money for those who desire to pursue multiple courses of study in the computational science and engineering arena. It will also offer students a coherent and consistent education with less duplication, and immerse them into interdisciplinary endeavor and a teamwork environment.

### Impact on Existing Academic Programs

The MS degree program in CSE builds upon the current University's curricular strength and research capability in science, engineering, mathematics, technology, and business. It is a result of interdisciplinary collaboration among the College of Arts and Sciences, College of Engineering, School of Agriculture and Environmental Sciences, School of Business and Economics, and the School of Technology. It will enhance and supplement current graduate research and education programs in science, engineering, mathematics, technology and business, and further the fertilizing and nurturing of cross-disciplinary interaction and collaboration in CSE among faculty and graduate students. As the first stand-alone CSE graduate degree program in the State of North Carolina and among HBCUs in the nation, the program will increase the eminence of North Carolina A&T State University in this keen technological area.

The graduate MS program in CSE will strengthen the other graduate and undergraduate programs in engineering, sciences, technology and business. Students in these programs will benefit from the new computational science and engineering courses. Computational methods have become an accepted and widely used solution methodology joining analytical and experimental techniques as the basic techniques in scientific, engineering research, design and applications. The new program along with the faculty, infrastructure resources and new courses will strengthen the undergraduate education and training by providing the undergraduate students access and experiences with these resources, research and educational activities. This exposure will influence and attract undergraduate students into this and other graduate programs in the University. The faculty and administration of the NCA&T feel strongly about the importance and effectiveness of undergraduate education. New interdisciplinary programs and research activities will further strengthen the undergraduate education and improve the quality and accreditation of undergraduate the undergraduate programs in engineering, science, technology and business. An established interdisciplinary Masters program should help recruit additional well-qualified faculty and students and simulate or enhance access to federal research funds. In turn, this will encourage our brightest and best undergraduates, as well as undergraduate students from other universities to consider our graduate programs.

The CSE Masters program is built upon our existing and new resources and dovetails of our FUTURES vision to promote an interdisciplinary learning and interactions across disciplines that the new and complex problems require. Many new emerging fields require interactions and expertise from multiple fields (for example: new developments in material sciences need understanding of both chemistry based atomistic material configurations and the associate mechanics and properties for the continuum level; bio-informatics need understanding of



genetics and computer science). The program leverages the existing resources and expertise to build a new interdisciplinary arena that strengthens, contributes and enhances the existing resources. The present graduate masters programs in engineering and sciences have the required enrollment and graduation rate that meets the productivity criteria. The interdisciplinary CSE graduate program will further enhance the productivity and graduate education in the university.

### University Benefits

The University will benefit in many ways from this new degree program. It will provide research and professional development opportunities for its faculty with collaboration with CSE master's students, CSE programs at other institutions, national labs and research centers, and high performance supercomputing community and industry. The program will attract students from a variety of disciplines with experience in industry, business, education, and government. The CSE program will also encourage enrollment of women and minority students such as Hispanics, Caucasians, Asian and Native Americans. The planning and development of the computational science and engineering program and the enrollment of diversified student population are directly linked to the University's Enrollment Plan to increase the population of graduate students, nontraditional students and working professionals, to increase participation of women in pursuing degree studies and career paths in science, engineering and technology, and to increase the presence of minority students on campus.

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