

Computational Science

John Wallin, Program Director
Wiser-Patten Science Hall (WPS) 217

The Computational Science Ph.D. is an interdisciplinary program in the College of Basic and Applied Sciences and including faculty from the departments of Biology, Chemistry, Computer Science, Mathematical Sciences, and Physics and Astronomy. This program is research intensive and applied in nature, seeking to produce graduates with competency in the following three key areas:

1. 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;
2. deep knowledge of programming languages and computing technology so that graduates can adapt and grow as computing systems evolve; and
3. skills in effective written and oral communication so that graduates are prepared to assume leadership positions in academia, national labs, and industry.

Requirements for the Ph.D. in Computational Science

Admission is based on a comprehensive assessment of a candidate's qualifications including Graduate Record Examination (GRE) scores, undergraduate and graduate grade point average, and letters of recommendation. Applicants must submit all application materials to the College of Graduate Studies.

Candidate must

1. submit application and fee to the College of Graduate Studies.
2. submit official transcripts showing a GPA in previous academic work that indicates potential for success in advanced study. Successful applicants typically have a minimum 3.5 GPA in their graduate work or a minimum 3.0 GPA when entering with a bachelor's degree. Applicants should hold a bachelor's, 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 may be required to participate in an intensive computational science leveling program before beginning their coursework.

3. submit official scores for the verbal, quantitative, and analytical writing measures of the 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 Verbal and Quantitative scores at or above the 50th percentile for persons intending graduate study in science with a combined V + Q score exceeding 1,000.
4. 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.

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, 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. Such students must meet the conditions of their admission in the time stated to remain in the program of study.

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.

Once admitted to the program, candidates must complete at least 72 semester hours as follows:

Foundation Courses (9 hours)

COMS	6100	Fundamentals of Computational Science
COMS	6500	Fundamentals of Scientific Computing
CSCI	6020	Data Abstraction and Programming Fundamentals

Computational Science Core (30 hours)

COMS	7950	Research Seminar in Computational Science
CSCI	7300	Scientific Visualization and Databases
CSCI	6050	Computer System Fundamentals Parallel Computing
STAT	7400	Computational Statistics
COMS	7100	Applied Computational Science
MATH	7450	Mathematical Modeling I

Electives (15 hours)

Three courses from the following, selected with the major professor and dissertation committee.

MATH	6270	Advanced Differential Equations II
MATH	6300	Optimization
MATH	7750	Mathematical Modeling I
CHEM	7720	Advanced Topics in Physical Chemistry
CHEM	7400	Computational Chemistry I
CHEM	7410	Computational Chemistry II
PHYS	7400	Computational Physics I
PHYS	7410	Computational Physics II
BIOL	6450	Advancements in Molecular Genetics
BIOL	6350	Biostatistical Analysis
BIOL	6390	Advanced Cell and Molecular Biology
BIOL	6760	Bioinformatics
CSCI	6100	Analysis of Algorithms
CSCI	6130	Selected Topics in Parallel Processing
CSCI	7350	Data Mining

Directed Research (6 hours before candidacy)

Dissertation (12 hours)

Students are also required to

1. make at least two research presentations at regional, national, or international meetings as the lead or coauthor;
2. be lead author or make significant contribution as coauthor of two articles published, in press, or under review in high quality, peer reviewed journals; and national, or international meetings as the lead or coauthor;
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.

Courses in Computational Science [COMS]

- 6100 Fundamentals of Computational Science.** Three credits. Prerequisite: admission to the Computational Science Ph.D. program or permission of instructor. Foundational overview of the mathematical and scientific underpinnings of computational science. Introduces the principles of finding computer solutions to contemporary science challenges. Offers preparation for core and elective courses in the Ph.D. program in Computational Science by reviewing essential mathematical methods and basic science principles drawn from biology, chemistry, and physics. Special topics include techniques of high performance computing and applications, parallel systems, and theory of computation, case studies in computational chemistry, physics, and mathematical biology.
- 6500 Fundamentals of Scientific Computing.** Four credits. Prerequisites: Graduate standing or permission of instructor. Fundamentals of problem solving approaches in computational science, including computer arithmetic and error analysis, linear and nonlinear equations, least squares, interpolation, numerical differentiation and integration, optimization, random number generations and Monte Carlo simulation. Students will gain computational experience by analyzing case studies using modern software packages such as MATLAB.
- 7100 Applied Computational Science.** Four credits. Prerequisites: Consent of instructor. Intense lecture and practice-based course in computational methods, with a research program offered. Possible topics include computational aspects of linear algebra; contemporary numerical methods (finite difference-based and boundary integral equation-based) for solving initial and boundary value problems for ordinary and partial differential equations arising in engineering, natural sciences, and economics and finance.
- 7300 Numerical Methods.** Four credits. Prerequisites: COMS 6500 or permission of instructor. Numerical methods for solving ordinary and partial differential equations, partial differential integral equations, and stochastic differential equations. Convergence and stability analyses, finite difference methods, finite element methods, mesh-free methods and fast Fourier transform are also included.
- 7950 Research Seminar in Computational Science.** Two credits. Prerequisites: admission to the Computational Science Ph.D. program or permission of instructor. Seminar course to build a broader understanding of problems and research topics in computational science through advanced reading of selected journal articles, group discussion, and presentations by both external and internal speakers in computational science.