

COMPUTATIONAL SCIENCE OFFERINGS at NCSSM

What is it?

Computational science is a new research methodology that uses mathematical models and simulations to study complex scientific problems. NCSSM is expanding its offerings and opportunities in this critically important area of science, looking to keep its students at the forefront of scientific knowledge and experience.

Course opportunities and suggested sequences

During the 2008-2009 school year, there are different suggested sequences for seniors and juniors:

Senior sequence (2008-2009 only):

Trimester	Course Number/Title	Prerequisites/Comments
First Trimester	IE 442* Research in Computational Science I	Strong preference for students who have completed IE416* Computational Chemistry or wish to start the computational biology (bioinformatics) videoconferencing class with Jackson Genomics Lab (Maine)
Second Trimester	IE 444* Research in Computational Science II	Continuation of Research in Computational Science (For some students Jackson Lab sequence continues)
Third Trimester	IE 446* Research in Computational Science III	Continuation of Research in Computational Science (For some students Jackson Lab sequence continues)

Junior sequence:

Trimester	Course Number/Title	Prerequisites/Comments
First Trimester	None	No courses available
Second Trimester	Computational Chemistry Seminar (90 minutes/week)	Good academic standing One beginning course in chemistry Permission of advisor
Third Trimester	Medicinal Chemistry Seminar (90 minutes/week)	Good academic standing One beginning course in chemistry Permission of advisor Computational chemistry seminar suggested
	IE 442* Research in Computational Science I	Students interested in computational chemistry research should have completed Computational Chemistry Seminar with at least a B average

Course Descriptions:

Computational Chemistry Seminar:

One trimester (0.5 units of credit)

Prerequisite: Completion of a basic chemistry course; good academic standing; permission of advisor

Meeting Pattern: One 90-minute session and approximately three (3) hours of out-of-class work per week

This seminar will provide students who have an interest in chemistry with the opportunity to learn the basic technologies, techniques, and tools of computational chemistry. The seminar consists of weekly lectures, quizzes, in-class and out-of-class labs. Upon completion, students will be able to describe basic computational chemistry methods and mathematics, and be able to solve a number of challenging chemical problems using a computational approach.

Medicinal Chemistry Seminar:

One trimester (0.5 units of credit)

Prerequisite: Completion of a basic chemistry course; good academic standing; permission of advisor; computational chemistry seminar strongly suggested

Meeting Pattern: One 90-minute session and approximately three (3) hours of out-of-class work per week

This seminar will provide students who have an interest in the health sciences (medicine, pharmacology, and allied health sciences) with the opportunity to use advanced computing methods in the study and design of medicinal compounds. The seminar provides an introduction to pharmacology, several sessions on drug design and optimization, and applications of pharmacogenomics to the drug design process. The seminar consists of weekly lectures, quizzes, in-class and out-of-class labs. Students interested in this seminar are strongly encouraged, but not required, to participate in the Computational Chemistry seminar as a prerequisite for this opportunity.

IE442* Research in Computational Science I

One trimester (1 unit of credit)

Prerequisite: Permission of the Dean of Science

Meeting Pattern: 4 periods per week including lab

This is an advanced course for first trimester senior students or third trimester junior students with the maturity, independence, and motivation necessary to conduct their own research project. Students learn computational methodology and design while conducting a variety of computational projects on a small scale. Students then write their own research proposals on a problem of interest to them. Throughout the semester students read from the primary scientific literature and participate in discussion groups on current issues in computational science research. Based on the outcomes of the semester's work, students may be given an opportunity to participate in summer research programs on campus or in the Triangle area. Students with a final grade of B or higher are encouraged to continue in IE442* Research in Computational Science II.

IE444* Research in Computational Science II

One trimester (1 unit of credit)

Prerequisite: Permission of the Dean of Science

Meeting Pattern: 4 periods per week including lab

In this course, students continue to conduct computational research based on their previous semester and/or summer work. Time is devoted to the completion of the research project and a written paper. Students are required to present their results at the NCSSM Research Symposium and at the NC Student Academy of Science competition. Students may, at their option, also enter their work in national competitions, where appropriate.

IE446* Research in Computational Science III

One trimester (1 unit of credit)

Prerequisite: Permission of the Dean of Science

Meeting Pattern: 4 periods per week including lab

In this course, students continue work on their previous research to produce additional data and analysis, as needed, or to research extension questions based on their original work. Students in this course have a leadership role in working with the junior students enrolled in IE442 Research in Computational Science I and may serve as teaching assistants.