

# SCIENTIFIC COMPUTING

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Many disciplines in the natural and social sciences include a significant sub-discipline that is explicitly computational. Examples include astronomy, biology, chemistry, economics, and physics. In some fields, such as biology, the use of computation has become so widespread that basic literacy in computation is increasingly important and may soon be required.

The Concentration in Scientific Computing gives students an opportunity to develop a basic facility with the tools and concepts involved in applying computation to a scientific problem, and to explore the specific computational aspects of their own major disciplines.

## LEARNING GOALS

As students progress through the curriculum, they will:

- learn to read, write, and debug code in at least one programming language, using idioms appropriate to the major field of study.
- apply computational reasoning to a broad set of problems.
- learn tools and concepts required to computationally approach scientific problems within the discipline of their major.
- appreciate trade-offs and limitations of computational approaches to problem solving (e.g., accuracy vs. computation time, approximations needed to make real-world problems calculable, numerical errors inherent to computations themselves).

## CURRICULUM

Three of the six courses required for the concentration focus on general issues of computing (see Requirements A and B below): two of these serve as an introduction to computer science and programming, and the third focuses on the use of computation within a specific scientific discipline. Students then choose the remaining three courses from a list of electives (see Requirement C), using at least two to connect their computational work with their major (recall that 2-3 courses for a concentration must also count toward the student's major). Finally, the student must also complete a project-based experience, possibly during the completion of one of the courses (Requirement D).

Students majoring in astronomy, biology, chemistry, economics, mathematics, and physics should consult the relevant sections of the Catalog for information about the relationship of this concentration to their courses of study.

Given the abundance of math, physics, chemistry, and computer science courses listed under Requirements B and C, students with these majors should have no problem choosing courses (though one of the coordinators of the concentration should be consulted during this selection). Example "Requirement C" tracks for majors in astronomy, biology, chemistry, and economics are available, but a student may of course choose other courses (in consultation with one of the coordinators).

## REQUIREMENTS

The concentration consists of six credits that fall into four categories of requirements, denoted (A), (B), (C), (D). These are merely categorical labels, and we have no intention of expressing a time-ordered sequence. In fact, we anticipate that many students in fields other than computer science will take at least one course in the (B) and/or (C) requirements before discovering an interest in the concentration, and then take courses to satisfy the other requirements afterward.

The six courses should be selected from the following list and approved by the student's concentration advisor. Of the six credits required for the concentration, no more than two of the courses in (B) or (C) may count towards both the concentration and the student's major. (Also, per College rules, students may not count among the 32 course credits required for graduation any course that substantially repeats the content of another course already completed, even though the course numbers may suggest an advancing sequence. For example, both introductory computer science courses, CMSC 105 and CMSC 110, cannot be taken for credit.)

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### Categories of Requirements

Category A: Year-long introduction to computer science and programming, that may consist of (CMSC 105 and CMSC 106) or (CMSC B110 and CMSC B206) or (CMSC 107).

Category B: One course involving regular programming assignments and becoming familiar with discipline-specific programming idioms, chosen from the following list:

- ASTR 341: Advanced Topics in Astrophysics: Observational Astronomy
- ASTR 342: Advanced Topics in Astrophysics: Modern Galactic Astronomy
- ASTR 344: Advanced Topics in Astrophysics: Computational Astrophysics
- CMSC 187: Scientific Computing-Discrete Problems
- CMSC 207: Data Science and Visualization
- CMSC 250: Computational Models in the Sciences
- CMSC 287: High Performance Scientific Computing
- CMSC/LING 325: Computational Linguistics
- CHEM 304: Statistical Thermodynamics and Kinetics
- CHEM 305: Quantum Chemistry
- MATH 222: Scientific Computing-Continuous Problems
- PHYS 304: Computational Physics

Category C: Three credits worth of electives in which real-world phenomena are investigated using computation, at a significant level as determined by the standards of that discipline. At least one of these three credits must come from a 300-level course or courses (not senior research). A normative route in the sciences would be for a student to take two taught courses on this list and apply one credit of senior research to this requirement. Alternatively, students whose senior work is not computational but who still wish to pursue the concentration can complete three taught courses from this list. These courses should be drawn from the following list:

- Any of the courses on the (B) list above
- BIOL 300: Superlab
- BIOL 301: Advanced Genetic Analysis (1/2 credit)
- BIOL 354: Computational Genomics (1/2 credit)
- BIOL 357: Protein Design (1/2 credit)
- CHEM 322: Advanced Physical Chemistry: Mathematical Modeling & Natural Processes

- CMSC 120: Visualizing Information
- CMSC 225: Fundamentals of Databases
- CMSC 235: Information and Coding Theory
- CMSC 250: Computational Models in the Sciences
- CMSC/LING 325: Computational Linguistics
- ECON 032: Operations Research
- MATH 204/210: Differential Equations, in years in which it includes significant computer lab exercises involving modeling and/or simulation
- MATH 210: Linear Optimization and Game Theory
- MATH 286: Applied Multivariate Statistical Analysis
- MATH 394: Advanced Topics in Computer Science and Discrete Math
- MATH 397: Advanced Topics in Applied Math
- MATH 056: Modeling
- PHYS 306: Mathematical Methods in the Physical Sciences
- PHYS 316: Electronic Instrumentation and Computers
- PHYS 026: Chaos, Fractals, Complexity, Self-Organization, and Emergence
- Up to 1 credit of senior research (e.g., ASTR 404, BIOL 40x, CHEM 361, CMSC 480, MATH 399, PHYS 41x), if the project has a significant focus on scientific computing

Category D: Some part of completion of the concentration must include a project-based experience in which computation is applied to investigate a real-world phenomenon, e.g.,

- A senior thesis/experience with significant scientific computing component, or
- A summer research experience, or
- A multi-week project for a course that may (or may not) be one of the three electives that fulfill requirement (C)

## CONCENTRATION COORDINATORS AND DEPARTMENTAL REPRESENTATIVES

### Robert Manning

Mathematics representative, William H. and Johanna A. Harris Professor of Computational Science

### Philip Meneely

Biology representative, Professor of Biology

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### **Joshua Schrier**

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representative, Associate Professor of Chemistry