

CMSC/AMSC 660-0101 TTh 9:30-10:45, CSI 3120

SCIENTIFIC COMPUTING I, Fall, 2008

<http://www.cs.umd.edu/users/oleary/c660/>

Prof. Dianne P. O’Leary: Room 3271 A.V. Williams Building, (301) 405-2678, oleary@cs.umd.edu, <http://www.cs.umd.edu/~oleary/>

Office Hours: Tuesday 1:00-2:15, Thursday 8:00-9:15, Friday 9-10, and by appointment, in AVW 3271.

Please restrict telephone inquiries to office hour times, except in “emergencies.” E-mail is welcome anytime!

Prerequisite: Undergraduate-level knowledge of numerical analysis: linear equations, nonlinear equations, integration, interpolation. Programming assignments will be in Matlab.

Text: Draft copy of *Scientific Computing: A Second Course, with Case Studies*, by Dianne P. O’Leary.

Topics: Monte Carlo simulation, numerical linear algebra, nonlinear systems and continuation method, optimization, ordinary differential equations. Fundamental techniques in scientific computation with an introduction to the theory and software for each topic.

News: Assignments, course notes, answers to homeworks and quizzes, and announcements will be posted on the course’s homepage. You are responsible for checking this site before each class.

Final Exam: None.

Grading: Grading will be on a *curve*, except that you will be guaranteed an A if your average is 90% or better, a B if your average is 80% or better, etc. Keep all of your work in case there is any question about recording of grades.

- **Homework:** 3 assignments, 120 points. To pass this course, you must make an honest effort at each homework. Partial credit will be given

for partially-working programs. There will be a 15% penalty for assignments turned in up to 2 days late, 30% penalty for assignments turned in 2-4 days late, etc.

- **Quizzes:** 140 points. Quizzes will be 20 minutes long, scheduled every third class. Make-ups will not be permitted unless you have documented medical or other serious excuses for more than two quiz dates. If there are no “snow days”, there will be 9 quizzes. The lowest two scores will be dropped.
- **Project:** 100 points. More information will be given in early November. It is due at 10am on Tuesday, December 16.
- **Extra Credit:** 0.5 points of extra credit (up to 20 points) will be given to the first student to find each error in the textbook. A free copy of the book will be given to the student who is credited for more than 40 errors and who finds more than anyone else in the class.

Note for Computer Science Department MS comp students: The MS Comp grade for this course is based on your best 7 quizzes.

Regrades: If you think a mistake has been made in grading your work, submit it for regrading within two weeks of the date on which the work was returned to the class. After that, the grade will be considered final.

Academic Integrity: Class accounts are to be used only for class assignments. All files within the accounts are subject to inspection, and the campus code of computer conduct must be followed. All work that you submit in this course must be your own; group efforts will be considered academic dishonesty. See <http://www.studenthonorcouncil.umd.edu/code.html> for definitions and sanctions. You may discuss homework in general way, but you may not consult any one else’s written work, program drafts, computer files, etc. Any marked similarity in form or notation between submissions with different authors will be regarded as evidence of academic dishonesty – so protect your work. You are free to use reference material to help you with assignments, but you must cite any reference you use and clearly mark any quotation or close paraphrase that you include. Such citation will not lower your grade, although extensive quotation might.

COURSE OUTLINE

1. Introduction, Computer Arithmetic and Errors (approx. 2 lectures)
 - course survey
 - machine arithmetic
 - error analysis
 - stability and conditioning
2. Matrix Factorizations (approx. 5 lectures)
 - Matrix manipulation
 - Matrix decompositions and their uses: LU, QR, rank-revealing QR, eigendecomposition, SVD
 - Updating decompositions
 - Software issues
3. Optimization (approx. 10 lectures)
 - unconstrained optimization: line searches and trust regions, Newton-like methods, conjugate gradients
 - constrained optimization: barrier methods, reduced-variable methods
 - simulated annealing, Metropolis algorithm
4. Nonlinear Systems and Continuation (approx. 3 lectures)
 - Newton-like methods
 - Globally-convergent homotopy methods
5. Monte-Carlo Methods (approx. 3 lectures)
 - basic statistics: random variables pseudo-random numbers
 - mean, variance, central limit theorem
 - basic Monte-Carlo simulation
 - Monte Carlo integration, convergence

- Monte-Carlo optimization
- variance reduction: stratified sampling, importance sampling

6. Ordinary Differential Equations (approx. 4 lectures)

- review of initial value problems for ordinary differential equations
- differential-algebraic equations
- boundary value problems