CMSC/AMSC 660-0101 Tuesday, Thursday 9:30-10:45 (CSI 2118)
SCIENTIFIC COMPUTING I, Fall, 2010
http://www.cs.umd.edu/users/oleary/c660/

Prof. Dianne P. O'Leary: Room 3271 A.V. Williams Building
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Office Hours: Tuesday 1-2:30, Friday 8:30-10,
and by appointment, in AVW 3271. E-mail is welcome anytime!

Teaching Assistant: Yun Zhou, zhouyun@math.umd.edu
Office hours: Monday and Wednesday, 9:30-11:30, MATH 3301.

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

Text: *Scientific Computing with Case Studies*, by Dianne P. O'Leary, SIAM Press, 2009

Topics: Monte Carlo simulation, numerical linear algebra, numerical solution of nonlinear systems and continuation method, optimization, numerical solution of 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.

Accommodations: If you require academic accommodations due to a religious obligation or a disability, you must provide documentation by the end of the 2nd week of the semester.

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 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.

CourseEvalUM: Please complete your evaluation for this course near the end of the semester at http://www.courseevalum.umd.edu.

COURSE OUTLINE

1. Introduction, Computer Arithmetic and Errors (approx. 2 lectures)

   - course survey
   - machine arithmetic
   - error analysis
   - stability and conditioning

2. Matrix Decompositions (approx. 5 lectures)

   - Matrix manipulation
   - Matrix decompositions and their uses: LU, QR, rank-revealing QR, eigendecomposition, SVD
   - Updating decompositions
   - Software issues

3. Optimization (approx. 8 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. 2 lectures)

   - Newton-like methods
   - Globally-convergent homotopy methods

5. Monte-Carlo Methods (approx. 2 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. 6 lectures)

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

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. At least 2 weeks will be allowed for each assignment. To pass this course, you must make an honest effort at each homework. Partial credit will be given for partially-working programs. Assignments will be due **before class begins**. 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. 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 mid-October.

- **Extra Credit**: There may be occasional opportunities during class to earn extra credit. Also, .5 point will be given to the first student to discover an un-found error in the textbook or the book's website.

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.