

MATH561 FALL 2016



SYLLABUS

COURSE:	SCIENTIFIC COMPUTING I
WEBPAGE:	http://math.duke.edu/~haizhao/Teaching/Math561.html
TIME/LOCATION:	MW - 11:45AM to 01:00PM in Physics 047
INSTRUCTOR:	Haizhao Yang, haizhao@math.duke.edu , Phys. Bld. 224 Office hours, Monday, 02:00 to 04:00 PM or by appointment
DESCRIPTION:	Numerical Linear Algebra, Optimization and Monte Carlo Simulation
RECOMMENDED TEXTS:	• <i>Iterative methods for sparse linear systems</i> – Yousef Saad. • <i>Convex Optimization</i>, Boyd and Vandenberghe, electronic copy available from http://stanford.edu/~boyd/cvxbook/. • <i>Matrix Computation</i> – Golub and Van Loan. • <i>Numerical linear algebra</i> – L.N. Trefethen and D. Bau. • <i>Papers recommended in class.</i>
IMPORTANT PREREQUISITES:	Students must review calculus and numerical linear algebra textbook in undergraduate courses by themselves. I strongly encourage you to review concepts like: matrices, vectors, matrix operations, matrix decompositions, eigenvalues and eigenvectors. Basic experience in programming in C/C++ or FORTRAN or MATLAB is also necessary (at the level of CPS 006 or higher). Other programming languages are allowed, albeit in this case the instructor may not be able to help with software/programming issues.
APPROXIMATE SCHEDULE:	An introduction to programming for scientific applications. The course focuses on efficient computational approaches to solve problems from linear algebra and nonlinear systems. Mathematical background is used to develop stable, reliable, accurate, and efficient numerical algorithms to be implemented in scientific programming language. Temporary list of topics: • Projectors, QR factorization; Gram-Schmidt orthogonalization; Newton-Schulz iteration; Spectral projector; Householder triangularization; least squares problems. • Singular Value Decomposition; randomized low-rank approximations.

- Linear systems; direct solver; iterative solver;
- Eigenvalue problem; direct diagonalization; iterative methods.
- Structured matrix factorization.
- Fast algorithms for applying structured linear operators; (nonuniform) fast Fourier transform, fast multipole method, butterfly algorithm.
- Basic convex optimization;
- Foundations of Monte Carlo algorithms: sampling, high-dimensional integrals, Metropolis algorithm.

GRADING:

► **Homework and Reading** – Weekly assignments based on encouraged readings. NOT a component of your final grade.

- A weekly assignment will be made in class and will generally not be placed in sakai. The assignment is only for the purpose of helping you understand the materials in class and it will NOT be graded. You are encouraged to work in groups on these homework problems.
- Half of the problems on the final exam will be taken from these questions.

► **Class Project** 60% – Find a class project related to the course content and match your background. Work in groups, each of which contains approximately 4 students. Starting from the third week, students in a group take turns to present a 8-minute slide in the office hour. Prepare for questions! A final presentation will be scheduled later in the end of this semester.

► **Final Exam** 40% – A in-class exam focused on conceptual materials .

NOTES/ EXPECTATIONS:

• Missed presentation work is officially accommodated in the following three circumstances:

1. Illness or other extraordinary personal circumstance:
<http://trinity.duke.edu/undergraduate/academic-policies/illness>
2. Religious observance
3. Varsity athletic participation

Makeup exams are not allowed. No notes are allowed in exams. All exams should be completed on your own.

- It is important that you understand and adhere to the Duke Community Standard (<http://www.integrity.duke.edu/standard.html>). Direct or indirect use of a solution manual either physical or online, either by a publisher or by some “random” individual, is not allowed and constitutes a violation of the Standard. If a student is found responsible through the Office of Student Conduct for academic dishonesty on a graded item in this course, the student will receive a score of zero for that assignment. If a student’s admitted academic dishonesty is resolved directly through a faculty-student resolution agreement approved by the Office of Student Conduct, the terms of that agreement will dictate the grading response to the assignment at issue.

- Working in groups on homework and to study is encouraged! Mathematics can be a wonderfully collaborative endeavour. However, please submit individual work, in your own words. Exams will be taken individually and are closed-notes/book.

- This is an advanced course with high expectations. Your submitted work should reflect your best effort. Solutions should be complete, legible, and easily understood. Complete sentences expressing well-developed ideas should be used whenever appropriate. We will compute, but we will also discuss and reflect. You must **understand** the meaning of bold-faced words in the text and the notes.

- THE GOAL OF THE COURSE IS FOR THE STUDENT TO HAVE A BASIC FEELING ABOUT SCIENTIFIC COMPUTING AND LEAVE THE CLASSROOM WITH EXPERTISE AT LEAST IN A SMALL FIELD.

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