Scientific Computing, I
Math 561

Dr. Mauro Maggioni
Office: 309 Gross Hall; 293 Physics Bldg.
Phone: 919-660-2825
Web page: www.math.duke.edu/˜ mauro
E-mail: mauro.maggioni at duke

Prerequisites

Mathematics 103 (multivariable calculus) and Mathematics 104 (linear algebra) or equivalents are needed for the mathematical background. Basic experience in programming in C/C++ or FORTRAN or MATLAB is also necessary (at the level of CPS 006 or higher). I strongly encourage you to revise basic linear algebra: matrices, vectors, matrix operations, matrix decompositions, eigenvalues and eigenvectors. Prior knowledge of any programming language (ideally C) is also a plus; we will be mainly using C and Matlab in this course, albeit use of FORTRAN, R, Octave, Python is allowed, albeit in this case the instructor may not be able to help with software/programming issues.

Detailed course content

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.

List of topics:

- Review of linear algebra: vectors, matrices, vector spaces, linear operators and their representations; orthogonal vectors and matrices; norms, inner products.
- Singular Value Decomposition; low-rank approximations.
- Projectors, QR factorization; Gram-Schmidt orthogonalization; Householder triangularization; least squares problems.
- Conditioning and stability; floating point arithmetic; stability of Householder triangularization, of back substitution, of least squares algorithms.
- Linear systems: Gaussian elimination, pivoting and stability. Cholesky factorization.
- Eigenvalue problems; Hessenberg and tridiagonal form; Raleigh quotient, inverse iteration, QR algorithm and its variations; Arnoldi and Lanczos algorithms.
- Iterative methods for linear systems: GMRES, conjugate gradient, preconditioning.
- Basic randomized algorithms in linear algebra: random projections, randomized SVD.
- Basic nonlinear optimization: bisection, Netwon's method, linear programs.
- Foundations of Monte Carlo algorithms: sampling, high-dimensional integrals, Metropolis algorithm.

Textbooks

- *Numerical linear algebra*, L.N. Trefethen and D. Bau.

Other references:

- *Scientific Computing, An Introductory Survey*, 2nd edition, by Michael T. Heath.

- *Matrix computations*, G.H. Golub and C.F. Van Loan.
- *Numerical recipes in C*, 2nd edition, by Press et al.
- *C Programming Language*, 2nd edition, by B. W. Kernighan and D. M. Ritchie; the classic on learning C.
- *Numerical mathematics*, Quarteroni, Sacco, and Saleri.
- *Scientific Computing* by John Trangenstein (lecture notes available on the web).

Assignments
Weekly problem sets will include theory, analysis and computational projects. A written solution and hardcopy of every code, input or output must be submitted for each problem. An electronic copy of our code must also be submitted to me via e-mail, in a unique zip or tar/gzip file. Requests for extensions on homework should be done before the due date; unexcused late assignments will not be graded. You are encouraged to discuss the homework problems with your classmates, but your final submission must be entirely your own independent work (see the Duke Community Standard).

Exams
Two exams. Grade to be based on weekly assignments (20%) and exams (80%). The final exam will include two parts: a take home exam focusing on algorithms and numerical experiments, and an in-class exam focused on conceptual materials.

Recommended Programming language: C/C++, Matlab, R; symbolic algebra: Maple; document preparation: LaTeX

Additional Information
Students from all areas of science, engineering, economics and quantitative studies that need advanced level skills in solving larger scale problems are encouraged to enroll. Scientific Computing II (usually taught in the Spring semester) continues this material and focuses on problems for integrals and differential equations.