COMPUTER SCIENCE 5485, 5486 (MATH 5485, 5486)
ADVANCED SCIENTIFIC COMPUTATION
(ADP TITLE: ADV SCIENTIFIC COMP)

I. CATALOG DESCRIPTION:

5485, 5486 (MATH 5485, 5486) ADVANCED SCIENTIFIC COMPUTATION

Presentation and analysis of numerical methods for solving common mathematical and physical problems. Convergence, error analysis. Hardware and software influences. Efficiency, accuracy and reliability of software. Robust computer codes. 5485: Methods of solving large sparse linear systems of equations, algebraic eigenvalue problems, and linear least squares problems. Krylov subspace and conjugate gradient methods. 5486: Numerical algorithms for solving constrained and unconstrained optimization problems. Numerical solutions of nonlinear algebraic systems and nonlinear least squares problems.

Pre: 5465 or (Math 4445 and Math 4446); (3H,3C) each. 5485: I. 5486: II.

II. LEARNING OBJECTIVES:

Having successfully completed this course, the student will be able to understand and apply advanced techniques in two major areas of computational methodology: computational linear algebra and analysis of nonlinear algebraic problems. The student will also be able to analyze important issues in scientific computation such as problem formulation and structure, the influence of high performance architectures, and the development and use of mathematical software.

III. JUSTIFICATION:

Large scale scientific computation has been made possible largely through the careful analysis of algorithm performance and exploitation of special structural features in the original problem formulation, taking into account factors such as numerical stability and effective utilization of high-performance computer architectures. This course will be of value to students within any curriculum having computational methodology as a significant component (to name a few - civil, mechanical, and electrical engineering, geophysics, engineering mechanics, and chemistry).

The course is addressed to students in their first or second year of graduate work having the basic knowledge and skills commensurate with successful completion of MATH 4445, 4446, (which itself may be taken for graduate credit) or CS/Math 5465. Furthermore, a variety of new abstract concepts fundamental to the course material are introduced that require a level of intellectual maturity undergraduates are generally not expected to possess. For these reasons, the 5000-level labeling of the course is felt to be justified.

IV. PREREQUISITES AND COREQUISITES:

Math 4445 and 4446, or CS/Math 5465 supply the necessary numerical analysis background and experience in basic scientific programming.

V. TEXTS AND SPECIAL TEACHING AIDS:

5485:

Golub, G. and C. Van Loan. MATRIX COMPUTATIONS. 3rd Edition. Baltimore: The Johns Hopkins University Press, 1996. xx, 644.

5486:

Dennis, J. and R. Schnabel. NUMERICAL METHODS FOR UNCONSTRAINED OPTIMIZATION AND NONLINEAR EQUATIONS. Philadelphia: SIAM, 1996. xvi, 378.

VI. SYLLABUS:

Percent of Course

5485:

1. Solution of Large Sparse Linear Systems — 45%
    a. Direct Methods
        1. LU, LDU, Cholesky factorization
        2. LAPACK, BLAS, and sparse matrix software
        3. Efficient use of data structures for the storage and factorization of matrices
        4. Reordering algorithms to reduce fill-in during factorization
    b. Iterative Methods
        1. Stationary methods, SOR, and SSOR
        2. Conjugate gradient methods and preconditioning
        3. Effects of computer architecture

2. Solution of Large Sparse Algebraic Eigenvalue Problems — 30%
    a. Transformation Methods
        1. The QL-QR methods and EISPACK
        2. Lanczos Methods and Krylov subspaces
    b. Iterative Methods
        1. Rayleigh Quotient interation
        2. Modified Lanczos methods and LASO
        3. Sturm sequences and bisection

3. The Linear Least Squares Problem — 15%
    a. Orthogonalization methods
        1. Updating factorizations with LINPACK
        2. Utilization of sparsity
    b. The singular-value decomposition
        1. Statistical interpretations
        2. Matrix pseudo inverses

4. Error Analysis and Mathematical Software — 10%
    a. Perturbation theory, numerical stability
    b. A priori and a posteriori estimates
    c. Robustness, reliability, portability of software
    d. Computational experiments for sensitivity

100%

5486:

1. Unconstrained Optimization and Systems of Nonlinear Equations — 30%
    a. Inexact Newton methods
    b. Line-search and model-trust region approaches
    c. Quasi-Newton updates
    d. MINPACK software

2. Nonlinear Least-Squares Problems — 20%
    a. Gauss-Newton method
    b. Levenberg-Marquardt method
    c. Large residual problems

3. Linear Constraints — 20%
    a. Reduced gradient methods
    b. Active set strategies
    c. Linearly constrained least squares problems

4. Nonlinear Constraints — 20%
    a. Projected gradient methods
    b. Augmented Lagrangian and penalty function methods
    c. Successive quadratic programming
    d. MINOS software

5. Global Methods for Nonlinear Equations — 10%
    a. Homotopy algorithms
    b. HOMPACK software

100%

VII. OLD (CURRENT) SYLLABUS:

5485:

Same as above.

<u>5486</u>:

Same as above.

VIII. CORE CURRICULUM GUIDELINES:

NA