Computazional Mathematics	Giovanni Russo	Suggested for students in Chemist, Physics, Engineering

The goal of the course on Computational Mathematics is to provide a basis on the methods used in the numerical solution of the various problems encountered in the mathematical modelization of natural phenomena. The course is transversal by nature, and it constitutes a bridge between the mathematical formulation of a problem and the possibility of obtaining quantitative answers.

The main objective is to provide the concepts at the basic of numerical computing, such as accuracy, stability and computational complexity of the methods and of the corresponding algorithms used in the quantitative solution of basic mathematical problems.

A second objective concerns the presentation of the modern methods for the problems that most frequently are encountered in applied science, such as the solution of linear systems of algebraic equations, nonlinear equations, computation of integrals, solution of ordinary differential equations.

A third objective is to teach how to use Matlab, a modern and effective computational tool, which quickly allows to solve several numerical problems in various fields.

The course is suitable for second year undergraduate students in Physics, Engineering, Chemists, Computer Science and Mathematics. The knowledge required to fruitful attend the course is rather modest. The theoretical lectures will be complemented with discussions on the most common applications of such methods to the various fields of interest for the students who attend the course.

Proposed progam

- Elements of programming in Matlab
  Vector and matrix operations. Graphical instructions. Elements of Matlab programming: cycles, conditions, functions.
- Error analysis:
  Representation of numbers on a given basis. Floating point representation. Machine numbers. Truncation and rounding. Machine operations. Propagation of errors.
- Numerical linear algebra:
  Summary of linear algebra: vectors, matrices and their properties. Vector and matrix norms. Eigenvalues, spectral radius, and relation with matrix norms. Direct methods for linear systems: triangular systems, Gauss elimination method, pivoting. PA=LU factorization. Conditioning in the solution of a linear system. Condition number. Iterative methods for linear systems: Jacobi, Gauss-Seidel, SOR. Convergence conditions. Stopping criteria. Conjugate gradient methods (hints). Sparse matrices and their representation. Solution of linear systems with Matlab. Applications of interest for the students. Least square method and applications.
- Interpolation and approximation:
  Polynomial interpolation in Lagrange and Newton form. Error formula. Chebyshev polynomials; recursive formulas, zeroes, minimum norm property. Interpolation by piecewise polynomials and spline functions. Computation of cubic splines. Approximation: Weierstrass theorem on the density of polynomials in C0 (statement). The problem of the convergence of a sequence of interpolatory schemes (hints). Bernstein polynomials. Interpolation and spline calculation with Matlab.
- Solution of nonlinear equations:
  General concepts. Bisection method, secant and tangent methods. General theory of iterative methods for nonlinear equations. Order of convergence. Stopping criteria. Newton's method for systems of non linear equations (hints). Minimization of functions. Method of the golden section. Non linear least squares (hints). Minimization using Matlab, and application.
- Quadrature formulas:
  General form of a quadrature rule. Polynomial order. Interpolatory formulas. Convergence theorem. Gaussian quadrature. Error estimation. Composite formulas: trapezoidal rule and Simpson's rule. Adaptive quadrature.
- Numerical methods for ordinary differential equations:
  Initial value problems. Recall of the theory of systems of ordinary differential equations (existence and uniqueness, continuous dependence from the data.) Forward and backward Euler method. One step method. Convergence, consistency and stability. Runge-Kutta methods. Order conditions of R-K. Explicit and implicit methods. Automatic step control. A-stability of R-K methods. Multistep methods (hints). Choice of the most suitable scheme. Numerical solution of ODE's with Matlab. Application to problems of interest for the students.
- Methods based on the Discrete Fourier Transform:
  The Fast Fourier Transform (FFT). Solution of the differential equations by FFT in one and two dimensions. Application to problems of interest for the students (e.g. solution of the Schrödinger equation for Chemists of Physics students, or problems of image digital filtering for computer science students).