LOGO DELLA STRUTTURA PRIMARIA

COURSE: Mathematics for Chemistry
ACADEMIC YEAR: 2016/17
TYPE OF EDUCATIONAL ACTIVITY: Basic
TEACHER: Occorsio Donatella

e-mail: donatella.occorsio@unibas.it	website:
phone: +390971205848	mobile (optional):
Language: Italian	

ECTS: (4 ECTS for lessons and 2 ECTS for tutorials/practice	n. of hours: (l36 hours for lessons and 24 hours for tutorials/practice)	Campus: Potenza Dept./School: Program:

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

In this course will be introduced basic elements in programming and in numerical computations.

The main goals:

Basic programming in Matlab. Numerical solutions of linear systems of equations, zeros of functions, approximation of eigenvalues and eigenvectors, best fitting by polynomials and approximation of functions by splines.

Final competences:

The student will be able to solve the assigned problem, by chhosing among different methods in order to obtain efficient procedures. “A priori” theoretical estimates of the erroprs are introduced.

PRE-REQUIREMENTS

Calculus

SYLLABUS

(10 h)Programming in Matlab

Basic algorithm and translation in Matlab

(5h) The machine arithmetic. Epsilon machine, absolute and relative errors, exact and significant digits. Stability of algorithms and condtioning of problems analysis.

(8h) Basic linear algebra.

Vector spaces. Algebra of Matrices . Linear algebra basic. Rank and determinant of a matrix.

(10 h) Numerical solution of linear system

Conditioning study. Gauss elimination . Partail pivoting. Inverse of a matrix.

(10h) Approximation of functions zeros

Bisection and Newton methods. Convergence order of iterative methods .

(7h) Numerical computation of eigenvalues and eigenvectors of a matrix

Power methos, Qr method.

(10h) Approximation of functions

Linear and cubic splines. Best fitting by polynomials. Error estimates .

LOGO DELLA STRUTTURA PRIMARIA

TEACHING METHODS Theoretical lessons: 36 hours, Laboratory tutorials: 24 hours. Personal training in numerical laboratory are provided.
EVALUATION METHODS Practical examinations in Matlab and oral examinations. The practical examination can be divided into two parts for regular attending student to Laboratory sessions. The oral examination in this last case can be skipped for student which have obtained 18/30 in mean at the two practical examinations.
TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL Notes by the teacher on the website of the degree course Istitutional book: *G. Monegato, Fondamenti di Calcolo Numerico, Edizioni C.L.U.T. Torino*
INTERACTION WITH STUDENTS Receiving schedule Monday 12.30 - 13.30 Tuesday 15 - 17 at the office 217 3d
EXAMINATION SESSIONS (FORECAST)[1] 15/02/2017, 15/03/2017, 21/06/2017, 19/07/2017, 22/09/2017, 21/12/2017
SEMINARS BY EXTERNAL EXPERTS YES □ NO X
FURTHER INFORMATION

[1]Subject to possible changes: check the web site of the Teacher or the Department/School for updates.