DIPARTIMENTO DI SCIENZE

COURSE: **MATHEMATICS FOR CHEMESTRY**			
ACADEMIC YEAR: **2018-2019**			
TYPE OF EDUCATIONAL ACTIVITY: Basic			
TEACHER: Prof. Incoronata NOTARANGELO			
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phone: +39 0971 205836		mobile (optional):	
Language: **Italian**			
ECTS: **6** (3 lessons and 3 tutorials/practice)	n. of hours: **60** (24 lessons and 36 tutorials/practice)	Campus: **Potenza** Dept./School: **Dipartimento di Scienze** Program: Chemestry	Semester: **I** (expected dates: from 01/10/2018 to 20/12/2018-20/01/2019)

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

- ***Knowledge and understanding.*** *Knowledge of basic elements of Scientific Computing, often used in Chemistry: basic programming in Matlab, elements of linear algebra, numerical mathods for linear systems, approximation of zeros of functions, approximation of eigenvalues and eigenvectors, method of least square, approximation of functions by splines.*
- ***Applying knowledge and understanding.*** *Using such mathematical tools and applying them for solving problems, studying the existence of solutions and their conditioning, and giving "a priori" error estimates.*
- ***Making judgements.*** *Choosing suitable numerical methods for solving problems.*
- ***Communication skills.*** *Using a proper mathematical language to express the knowledge in oral and written form. Justify the choice of the method for solving theoretical and application problems.*
- ***Learning skills.*** *Learning the contents of the course and relating them to other topics in the Program of Studies. Using the suggested books for exercises, insights and comparisons.*

PRE-REQUIREMENTS

Calculus.

SYLLABUS

- ***Programming in Matlab*** *(10 h)*

Basic algorithm and translation in Matlab.

- ***The machine arithmetic*** *(4 h)*

Machine epsilon, absolute and relative errors, exact significant digits. Stability of algorithms and conditioning of problenms analysis.

- ***Basic linear algebra*** *(12 h)*

Vector spaces.Spazi vettoriali. Algebra of matrices. Systems of linear equations. Rank and determinant of a matrix.

- ***Numerical mathods for linear systems*** *(10 h)*

Conditioning study. Forward and backward substitution for triangular systems. Gauss elimination method. Partial pivoting. LU factorization and inverse matrix.

- ***Approximation of function zeros*** *(8 h)*

Misection and Newton methods. Convergence order of iterative methods.

- ***Numerical computation of eigenvalues and eigenvectors of a matrix*** *(8 h)*

Localization of eigenvalues. Conditioning of eigenvalue problems. Power method. QR method.

- ***Approximation of data and functions (8 h)***

Method of least square. Approximation of functions by splines.

TEACHING METHODS

The course consists in 24 hours of lessons and 36 hours of tutorials/practice (with theoretical excercises and pratical training in numerical laboratory).

EVALUATION METHODS

Pratical-written test and oral examination.
The aim of the examination is to test the level of achievement of the previously mentioned educational goals.

The exam is divided into 2 parts:

- a pratical-written test using Matlab containing theoretical and application exercises on all the topics covered in the course; the test is indended to evaluate the knowledge and unterstanding of the topics and is selective (the student who does not show sufficient knowledge of the subjects is not admitted to the oral examination). To pass the test one must obtain at least 16 points out of 30. The expected time for the test is 2 hours. During the test the use of books, notes or smartphone is forbidden.
- an oral examination (to be taken during the same exam session of the written test) which will evaluate the ability to link and compare different topics of the course and will consist in the discussion of the written test, some theoretical questions and eventually short exercises. After this examination, the student will receive a final grade: in order to pass the exam this grade shold be at least 18 out of 30; otherwise, one shold repeat both the pratical-written test and the oral examination.

Students who attend the lectures may take optional intermediate written tests with theoretical and pratical exercises on specific part of the program.

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

Teaching material provided by the teacher, avalaible at https://sites.google.com/site/inconota/

Textbook: *G. Monegato, Fondamenti di Calcolo Numerico, Edizioni C.L.U.T., Torino, 1998.*

INTERACTION WITH STUDENTS

At the beginning of the course goals, program and evaluation method will be described.
At the end of the discussions of each topic the teacher provides the related teaching material in the web page of the course.
Office hours: Thursday from 14.30 to 16.30, office n. 63/3D214 of DiMIE (building 3D, second floor).
In addition to the weakly office hours, the teacher is avalaible everyday via e-mail.

EXAMINATION SESSIONS (FORECAST)[1]

15/02/2019, 01/03/2019, 27/06/2019, 09/07/2019, 03/09/2019, 01/10/2019, 20/12/2019

SEMINARS BY EXTERNAL EXPERTS YES □ NO ✓

FURTHER INFORMATION

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