Computational Chemistry and Classical Molecular Dynamics

Chemistry and Biochemistry

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Course Intro: : This course introduces learners to elementary programming and numerical methods that are useful to solve problems in chemistry. These methods are useful for understanding molecular structures as well as condensed media such as liquids and solutions. For rapid calculations, the public domain software Scilab is used and applications to several numerical methods relevant to chemistry are discussed. Basic mathematical background is provided wherever necessary. Classical molecular dynamics simulations are performed using the public domain software gromacs. Installation procedures as well explicit calculations are demonstrated. All these calculations can be performed on a personal computer.

Pre Requisites: : Good high school education. Thermodynamics in Bachelors courses will help
Core/Elective: : Both
UG/PG: : Both
Industry Support : Any pharmaceutical company will find this useful

Reference : NPTEL web course on computational chemistry

About Instructor: Ph. D in theoretical chemistry /chemical physics from Stony Brook University, 1981. Have taught physical/theoretical/computational chemistry and researched in these areas for nearly 40 years

COURSE PLAN

SL.NO	Week	Module Name
1	1	General Introduction and course outline
2	1	Algorithms Simple programs and the sine function
3	1	Flow charts, recursion relations and convergence and do loops
4	1	Branching and if statement. Solving a quadratic equation
5	1	Quadratic equation, dimension statement
6	1	Reading and writing from files
7	2	Execution of simple programs-1
8	3	Program execution 3
9	4	Integration
10	5	Scilab 4
11	6	Gromacs files-1
12	7	Results for liquid argon
13	8	Correlation functions-1