TCIS, Hyderabad

Course: Numerical Methods and Algorithms in Chemical Physics
Start Date: March 2021
Coordinates: Tuesday and Thursday between 11.30 am and 01.00 pm (preferred)
Instructor: Dr. Raghunathan Ramakrishnan (ramakrishnan@tifrh.res.in)
Teaching Assistant: Mr. Saurabh Chandra Kandpal (sckandpal11@gmail.com)

Syllabus:

1) **Python:** Writing/running codes: Editors, Ipython; modules, matplotlib, numpy
2) **Linear Equations:** Gaussian elimination, LU decomposition, Direct/Iterative methods
3) **Curve Fitting:** Least squares fitting, polynomial interpolation, splines
4) **Root finding:** Graphical, bisection, Newton-Raphson
5) **Numerical Differentiation:** Finite difference; Error analysis
6) **Numerical Integration:** Newton-Cotes formulae, Romberg/Gaussian integration, Multiple integrals
7) **Initial Value Problems:** Euler/Runge-Kutta methods; Stability and Stiffness
8) **Boundary Value Problems:** Shooting Method
9) **Symmetric Matrix Eigenvalue Problems**: Jacobi rotations, Power/inverse power method, Tridiagonal form
10) **Minimization/Optimiztion:** 1-D problems, N-D problems, Powell's method, Simplex method
11) **Application to Chemical Physics:** Molecular thermodynamics (Ideal gas, harmonic oscillator, rigid rotor partition functions), Equation of states, Schroedinger equation of Hydrogen molecule cation, Hartree-Fock for He atom, Linear variational problems in Quantum mechanics (1D potentials, Tunneling problems), Potential energy surface fitting, Time-dependent Schroedinger equation.
12) **Optional Topic:** Krylov Subspace Techniques, Lanczos iteration

Required Text

1. *Numerical Methods in Engineering with Python 3,* Jaan Kiusalaas, Cambridge university Press (2013).

Evaluation Method:
Quizzes based on assignment (4x10%), closed-book mid-term exam (30%), closed-book final exam (30%).