CHM684A
Computer Programming for Chemistry

First course handout

Instructor: Mainak Sadhukhan

Indian Institute of Technology Kanpur

January, 2023

Space-time coordinates

Venue: New core lab computer laboratory (Room 101A)

Timing: Monday (9 AM), Wednesday (9 AM), Friday (9 AM)

Exam dates: As per DOAA calender

Topics to be covered

Plotting is considered as an integral part of the course.

- Whys and hows of scientific computations: Languages, compilers and programming models
- Modern fortran versus python: When to use and how to use.
- Numerical algebraic methods: Roots of algebraic equations, System of linear equations, numerical diagonalization, optimization algorithms
- Finite difference methods: Numerical differentiation and integration and their applications to differential equations.
- Discrete Fourier transform
- Examples will be drawn from Monte Carlo, Molecular dynamics, Nonlinear dynamics and Electron structure theory problems amongst others
- Parallel programming with MPI libraries

Grading policy

- Regular assignments will be given and will cover 40% marks
- There will be no mid-semester examination
- Two group projects will cover 20% marks each
- End-semester examination will cover 20% marks
- No prorating is admissible in any circumstances.
- End-semester make-up examination can only be admissible for medical emergency, properly approved by authorities (SPGC/SUGC)

References

Books

1. Computer Programming in Fortran 90 and 95, V. Rajaraman,Prentice Hall India Learning Private Limited
2. Modern Fortran Explained: Incorporating Fortran 2018 (Numerical Mathematics and Scientific Computation), Michael Metcalf, John Reid, Malcolm Cohen, OUP Oxford; 5th edition
3. Numerical methods for scientists and engineers, Richard W. Hamming, Dover publications
4. Scientific Computing with Python: High-performance scientific computing with NumPy, SciPy, and pandas , Claus Fuhrer , Jan Erik Solem , Olivier Verdier, Packt Publishing Limited

Online resources

The instructor will mention possible online resources during teaching.

Contact informations

Office: Office 4, C' block, Old-SAC complex
Email: mainaks@iitk.ac.in
Phone: 0512-259-2062
Homepage: `http://home.iitk.ac.in/~mainaks`

The students are very much encouraged to contact the instructor whenever needed