TOOLS IN SCIENTIFIC COMPUTING

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TYPE OF COURSE	: New I Elective I UG/PG
COURSE DURATION	: 8 weeks (18 Jan'21 - 12 Mar'21)
EXAM DATE	: 21 Mar 2021

PRE-REQUISITES : 1st year undergraduate mathematics, Partial Differential equations

INTENDED AUDIENCE : Undergraduate and postgraduate students

INDUSTRIES APPLICABLE TO : This is expected to be a basic course which would enable the student to undertake research and development with the help of freely available scientific tools. It is difficult to pinpoint which industry would find value in this course.

COURSE OUTLINE :

Rapid advancements in computer hardware and high quality software libraries have enabled one to undertake works requiring high precision scientific computing with relative ease. The course involves exploration of various tools available for scientific computing with an emphasis on hands-on implementation. The course will deal briefly with the theory and the associated implementation for practical problems that an engineer may encounter. Undergraduates, postgraduates, and PhD students may find this course immensely useful for their project or research work. The course will make use of Python, GNU Octave, and PETSC (C based) as the medium of coding.

ABOUT INSTRUCTOR :

Aditya Bandopadhyay received his Dual Degree (Institute Silver Medal) from the Department of Mechanical Engineering, IIT Kharagpur in 2012. After receiving his Ph.D. from IIT Kharagpur in 2015, he was a postdoctoral researcher in CNRS Geosciences, France and a Humboldt fellow in TU Darmstadt. He joined IIT Kharagpur as an Assistant Professor in 2017. He became an Associate of the Indian Academy of Sciences in 2018. His areas of research span Fluid Mechanics across microscale and geophysical scales, and electrohydrodynamic phenomena. He was awarded the INSA Medal for Young Scientists in 2020.

COURSE PLAN :

Week 1: Introduction to numerical methods-discussion on techniques studied in other NPTEL courses and relevance to science and engineering.
Some basic ideas revisited - numerical errors, round off errors
Elementary demonstrations of using computer programs for system of linear equations, nonlinear algebraic equation etc. using Python/GNU Octave

Week 2: Nonlinear dynamics - 1D and 2D flows (Python, GNU Octave)
Understanding flows in 1D and 2D
Understanding phase portraits and the structure of nonlinear ODEs

Week 3: Nonlinear dynamics contd. Logistic maps and Time dependent ODEs using Python/GNU Octave

Week 4: Random walks, Probability distribution functions, and stochastic processes using Python/GNU Octave

Week 5: Boundary value problems
Ideas of regular and singular perturbation methods and implementations in Python/GNU Octave

Week 6: Finite difference methods for PDEs using PETSC

Week 7: Finite difference methods for Convection-diffusion problems

Week 8: Tools for experimentalists (GNU Octave/Python)