ALGORITHMS FOR PROTEIN MODELING AND ENGINEERING

PROF. PRALAY MITRA

Department of Computer Science and Engineering
IIT KGP

TYPE OF COURSE : New | Elective | PG
COURSE DURATION : 12 Weeks (26Jul 21 - 15 Oct 21)
EXAM DATE : 23 Oct 2021

PRE-REQUISITES : Preliminary knowledge of programming.

INTENDED AUDIENCE : Senior BE/BTech students, Master's students, Ph.D. students, Facultymembers, Professionals from Industry. All those whowish to learn and apply their knowledge in either teaching or research on bioinformatics, health care, medical science, pharmacology, drug discovery, etc. Computer Science and Engineering, Chemical Engineering, Electronics & Electrical Communication Engineering, Electrical Engineering, (v) Agricultural and Food Engineering, Civil Engineering, Biotechnology, Physics, Chemistry, Mathematics, School of Medical Science and Technology, and School of Bioscience.

INDUSTRIES APPLICABLE TO : Drug design industries like Novartis, Astrazeneca, Dr. Reddy's Laboratories, Bharat Biotech International Limited who are working on drug design and pharmacology may recognize this course.

COURSE OUTLINE :
Proteins are responsible for almost all the functions of the living organism including humans. Understanding proteins interactions and functions helps us to understand disease initiation, progression, and aids in drug design. In this regard Bioinformatics, an interdisciplinary area that deals with designing algorithms for biological problems, is a well-established alternative of cost and resource intensive experimental techniques. In this course we shall discuss the algorithms behind the existing Bioinformatics software tools for protein modeling and engineering so that customization of those software can help us to improve applicability. We shall also discuss some of the unique computational challenges and open areas, solving which can significantly improve human life.

ABOUT INSTRUCTOR :
Pralay Mitra is an Associate Professor of the Department of Computer Science and Engineering, Indian Institute of Technology Kharagpur. He did his Ph.D. from the Indian Institute of Science Bangalore in 2010 and was a postdoctoral researcher at the University of Michigan, Ann Arbor (from 2011-2013).Dr. Mitra is actively working on Bioinformatics and Computational Biology. Over the years, he developed expertise in modeling and designing protein structures and protein functions. He has developed several algorithms for protein-protein docking, predicting protein assembly from the crystal structures and protein design.

Further details can be found at personal webpage:
http://cse.iitkgp.ac.in/~pralay/index.html
http://www.iitkgp.ac.in/department/CS/faculty/cs-pralay

COURSE PLAN :

Week-1: Introduction
Week-2: Algorithmic techniques for modeling
Week-3: Algorithmic techniques for modeling (Contd.)
Week-4: Algorithmic techniques for modeling (Contd.)
Week-5: Application of REMC and SA on the protein folding problem
Week-6: Protein-protein interaction prediction

Week-7: Protein-protein interaction prediction (Contd.)
Week-8: Protein-protein interaction prediction (Contd.)
Week-9: Algorithm to infer protein assembly in crystals

Week-10: Algorithmic techniques for protein design and engineering
Week-11: Protein design and engineering
Week-12: Role of a score function in protein engineering