Title of the course: Computational Biophysics: Algorithms to Applications (CS61060)

Credit requirement: (L-T-P: 3-1-0, Credit: 4)

Objective: The objective of this course is to prepare the students for the field of computational biophysics and bioinformatics working either in research or in industry. Therefore, it is developed to introduce the most important and basic algorithmic concepts in biophysics. Emphasis will be given on understanding and utilizing existing algorithms to solve protein/nucleic acid related biophysical problems. No prior knowledge of biology/biophysics is required. There is no prerequisite for this course.

Content:

Introduction (Lecture hours: 3): Central dogma of molecular biology, Relevant databases in computational biophysics, Molecular visualization software.

Algorithmic techniques for modelling (Lecture hours: 9): Monte Carlo simulation, Replica-Exchange Monte Carlo simulation, Simulated Annealing, Neural Network method.

Protein/nucleic acid structure modelling (Lecture hours: 9): Methods for protein secondary structure prediction, Comparative modelling, Threading and fold recognition, Ab initio modelling, Combined modelling approaches, CASP: A blind protein structure prediction competition.

Protein-protein/nucleic acid interaction prediction (Lecture hours: 9): Fast Fourier Technique, Geometric hashing, Designing scoring function, Protein-protein docking algorithms, Protein-nucleic acid docking methods, CAPRI: A blind protein interaction prediction competition.

Selected topic (any one of the followings will be covered) (Lecture hours: 5):
(i) Protein function annotation: Gene ontology, Enzyme classification, Sequence and structure-based function annotation, Meta Servers.
(ii) Protein Design: Force Field Design, Simulation Techniques, Ab initio design, Interaction Design

Text Book:

1. Neil C. Jones and Pavel A. Pevzner. An Introduction to Bioinformatics Algorithms.
2. Gary D. Stormo. Introduction to Protein-DNA Interactions: Structure, Thermodynamics, and Bioinformatics.
3. Bruce R. Donald. Algorithms in Structural Molecular Biology (Computational Molecular Biology).

Literature:

1. Christopher M. Dobson, Andrej Sali, Martin Karplus. (1998) Protein Folding: A Perspective from Theory and Experiment. *Angewandte Chemie International Edition* 37(7):868-893.
2. Inbal Halperin, Buyong Ma, Haim Wolfson, Ruth Nussinov. (2002) Principles of docking: An overview of search algorithms and a guide to scoring functions. *Proteins: Structure, Function, and Bioinformatics* 47(4):409-443.
3. Joan-Emma Shea and Charles L Brooks III. (2001). FROM FOLDING THEORIES TO FOLDING PROTEINS: A Review and Assessment of Simulation Studies of Protein Folding and Unfolding. *Annual Review of Physical Chemistry* **52**:499-535.