Shubh Maheshwari 2016170

RnD Showcase Report

(1) Prediction of Protein Secondary Structure

Authors: Vineeth Chelur, Dr. V. Deva

The primary aim of the paper is to accurately predicted the 3D structure of a protein structure using the sequence of the molecules. The problem was divided into classifying the amino acid which constituted the Protein.

Bidirectional LSTM were used to predict the amino acids. They result in 84% due to stability of on learning how to predict long temporal sequences. The theoretical accuracy stands between 88-90%

5789 proteins with a sequence similarity cut-off set at 25% and X-ray resolution of 2.0 Å was used from FASTA dataset. Grension toolkit was used to create a vector space to achieve 70% accuracy.

Future work: Building 3D structure of the protein more precisely.

(2) Fast DFT Simulation of Argon

Author : Punyaslok Pattnaik, Tarun Kalluri, C.V. Jawahar, Prabhakar Bhimalapuram & Dr. Deva Priyakumar

The primary aim of this paper was to predict the solid facts of argon from the traditional discrete fourier transform methods.

The goal of the work to use DFT based methods on smaller system and replicate the results on larger systems. Classical force fields provide good simulations but are weak on accurately predicting properties.

DFT simulations are not feasible for large systems. Poison based sampling was used to generate random environment configuration.