Understanding Interaction Potentials for Coarse Grained Polymer MD Simulations

INTERNSHIP REPORT

SUBMITTED TO:

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I, **Preeti Parnna** from **Parala Maharaja Engineering College**, sitalapalli (Berhampur, Odisha) have done my one month internship organized by **TEQIP-3** under the guidance of **Dr. Balaji Iyer**. I have completed my internship on the topic ***'Understanding interaction potentials for the coarse grained polymers MD simulations'*****.**

ABOUT TOPIC:-

- Coarse grain techniques, such as united atom model applies various length and time scales for simulation of polymer systems. The interatomic force field is based on united atom model which uses Dreiding potential.

- The Dreiding potential determines the interactions between united atoms. It has four contributing terms; bond stretching, changes in bond angle, changes in dihedral rotation, and van der Waals non-bonded interactions.

- The interaction potential has two components which are summed over all possible atom combinations: bonded and non-bonded interaction terms.

- We required different parameters in the form of small segments. Plotting of these small segment manually is time consuming and difficult. Hence, plotting graphs for varied parameters of different Interaction potentials is required to know the force field effects.

- It also tracks the effects of other internal structure: chain end-to-end distance, polymer density, chain radius of gyration and chain orientation.

- It was a great opportunity to explore our knowledge and gain skills and experience of working on a major project which will help us in our near future.

- I have completed this program successfully due to coordination and cooperation of all the TEQIP team , IIT HYDERABAD staffs and my guide Dr. Balaji Iyer Sir.