AICTE QIP Short Term Training Programme

on

Applications of Molecular Simulations and Machine Learning in Research

March 21 - 26, 2022

Coordinators

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Sponsored by

All India Council for Technical Education

Organized by

Department of Chemical Engineering
Indian Institute of Technology Madras

Theme of the course:

Molecular modeling and simulation allow us to calculate macroscopic properties of a system from the knowledge of microscopic details such as forces of interactions. In other words, it is a mathematical way of mimicking the behavior of a collection of molecules. The simulation techniques can be broadly classified into two categories: Molecular Dynamics (MD) and Monte Carlo (MC). MD generates the trajectory (coordinates as a function of time) of a system of molecule as it goes from an initial state to the corresponding final state. From these trajectories, one can measure time-averages of properties of interest. Contrastingly, MC samples the phase space with an underlying distribution dictated by statistical mechanics, and one measures properties averaged over an ensemble of microstates of the system. Moreover, machine learning has remarkable ability to classify, recognize, and characterize complex patterns and trends in large data sets, and help in accelerating molecular simulation and improve the accuracy of molecular simulation-based property calculation. Integration of these two tools - molecular simulation and machine learning - can accelerate materials design and development.

Objective and scope:

The objective of this course is to disseminate principles of molecular simulation and machine learning techniques and show how these two tools can be used to compute and predict materials properties. The course will highlight best practices, key challenges, and important advances in molecular model development, simulation techniques, advanced sampling methods, use of machine leaning for data analysis. Participants will learn ways to improve and validate the prediction of molecular simulations and machine leaning, usefulness of these tools in materials research and education.

Course content:

THEORY & MODEL BUILDING

- Length and time scale analysis
- Theory of MD and MC
- Model building for MD and MC
- Discussion on potentials; force fields
- Running MD in NAMD, VMD
- Property Calculations from MD and MC simulation
- Introduction to Machine Learning
- Molecular Simulation data analysis via Machine Learning
- Materials Design using Machine Learning and Molecular Simulation

APPLICATIONS

- Structure & Dynamics of polymer melts
- Phase behavior of colloidal suspensions
- Protein ligand binding
- Transport through ion channels
- Mechanical properties of nanocomposites
- Mineral organic interaction in biocomposites
- Calculation of polymer phase diagram using Machine Learning
- Supervised Machine Learning for the design of stabilizers
- Genetic Algorithm for the design of inhibitors for protein aggregation

COURSE DURATION & VENUE

The course is of six days duration from **March 21 - 26, 2022**. Classes will be held online.

ELIGIBILITY

The course is open to faculty with background in Chemical Engineering, Chemistry, Metallurgy & Materials Science, Mechanical Engineering and Biotechnology from engineering colleges approved by AICTE. ***Participants from academic institutions, both from AICTE approved and other colleges: ₹ 1,000.***

For the first 30 college teachers from AICTE approved colleges the registration fee will be refunded after the course is completed.. For other participants, the fee is ₹. 10,000.

USEFUL LINKS

Course page: https://che.iitm.ac.in/molsim/
Center for Continuing Education, IITM: http://www.cce.iitm.ac.in/
Department of Chemical Engineering, IITM: http://www.che.iitm.ac.in/
Course coordinators Profile:
Dr. Ethayaraja Mani; https://che.iitm.ac.in/ethaya
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