

A Virtual Winter Workshop on Advanced Molecular Dynamics Simulations

Tentative dates:
06th - 17th September 2021

This workshop aims at introducing graduate students, young researchers and early career faculties from basic to advanced concepts of MD simulations and introductory sessions on machine learning and scientific renderings related to Bio-Physics. This workshop is divided into two weeks. The first week of the workshop is mainly focused on the basics of MD, a variety of computational software and uses of HPC facilities as well as a special session on 3D rendering via "Blender" software, and other necessary training to handle the advanced lectures to follow on the second week of the workshop. The latter is focused on MD simulations with the interpretation of results and introduction to some post-processing techniques.

The morning sessions of the workshop will consist of lectures on the basic principles and methodologies followed by a special lecture or research talks (covering experimental and theoretical aspects) showing their applications. The afternoon sessions will consist of hands-on tutorials where the participants will do simple and advanced calculations using the GRoningen MAchine for Chemical Simulations, and an introduction session to Machine Learning techniques. Further, the school provides access to HPC facilities (both CPU and GPU architecture) for a month to familiarize and train themselves with the concepts taught in the workshop.

Recommended System Configuration



RAM: 8 GB
STORAGE: 30GB (Atleast)
OS: 64 bit with virtualization support



Additional Requirements:

1. Good wifi (Ethernet recommended)
2. Windows users "C-Drive" should have Atleast 20GB Free Space else Install VirtualBox in other Drive

Applications

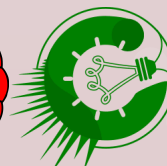
GROMACS patched with PLUMED
WHAM
CHARMM
Quantitative structure activity relationship (QSAR)
Auto-dock VINA/ADFR/MGL tools

FFPARAM/VMD/CHIMERA
BLENDER
CP2K/QE
Introduction to ML

**One project on 3D rendering and
another project on MD simulations.**

Registration link:
<https://tinyurl.com/AMDS2021>

Organizers:



Scidart Academy

The International School of Photonics,
Cochin University of Science and Technology (CUSAT), India

Department of Physics, & the Green Club of Thoughts,
Kathmandu University, Nepal