Molecular Dynamics Setup, Equilibration & Production — Hands-on

Learn how to convert parameterized biomolecular systems into stable, production ready molecular dynamics simulations. This module focuses on minimization strategies, staged equilibration (NVT and NPT), thermostat and barostat choices, and robust production run setup so that you obtain physically sensible trajectories suitable for downstream analysis and free energy workflows.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

MD Basics, Inputs & Pre Run Checks

Molecular dynamics concepts and integration basics

equations of motion idea **time step and stability** **constraints and rigid bonds**

MD input files, topology and coordinate sanity checks

topology and parameter linkage **box vectors and periodic boundaries** **energy minimization test run**

idea

Non bonded setup and neighbor list concepts

short range cutoffs | long range electrostatics overview | list update and performance notes

Session 2

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Energy Minimization & Restraint Schemes

Energy minimization strategies before dynamics

steepest descent idea | convergence criteria and maximum steps | fixing common initial clashes

Position restraints and soft start protocols

restraining heavy atoms and backbone | gradual release of restraints | handling ligands and cofactors carefully

Short restrained MD to relax solvent and side chains

relaxing water and ions first | monitoring energy and temperature trends | criteria to move into full equilibration

Session 3

Fee: Rs 14800 Apply Now

NVT/NPT Equilibration & Production Design

NVT and NPT ensembles and when to use them

constant volume vs constant pressure | density stabilization idea | typical step wise schedules

Thermostats, barostats and coupling parameters

temperature coupling schemes overview | pressure coupling and compressibility | relaxation times and

stability

Designing production runs and basic monitoring

trajectory length and sampling goals | output frequency and file sizes | on the fly checks for crashes and drift

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Reproducible MD Setup

Define system, ensemble and MD protocol for a chosen target

Theory + Practical

Run minimization, staged equilibration and short production test

validate basic thermodynamic stability | check energy and temperature profiles | prepare final production configuration

Deliverables: MD parameter set, logs and protocol report

simulation input and run scripts | summary of equilibration behaviour | steps to reproduce on another system