Advance Molecular Dynamics Simulation

Trajectory Analysis

From raw simulations to mechanistic insight — Visualization, Kinetics, Allostery, Enhanced Sampling, and Reproducible Research Workflows.

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PROGRAM CURRICULUM

Five Days · Five Dimensions of MD Analysis

DAY 1

Visualization & Trajectory Fundamentals

TOPICS

VMD · ChimeraX · Frame navigation · Alignment · Movie-making

LAB

Load a protein trajectory; clean movie; figure panel

Inspect trajectories confidently; export publication-quality visuals

DAY 2

Stability, Flexibility & Local Interactions

TOPICS

RMSD · RMSF · Rg · SASA · H-bonds · Contact maps · MDAnalysis

LAB

Analyze protein–ligand trajectory; plot time series; compare replicas

Full stability report with plots and interpretation

DAY 3

Global Motion & Conformational Landscapes

TOPICS

DCCM · PCA · dPCA · TICA · Clustering · Free-energy surfaces

LAB

Build feature sets; perform PCA/TICA; cluster frames; project to FES

Identify major conformational states and dominant motions

DAY 4

Function, Allostery & Binding Mechanisms

TOPICS

Dynamic networks · Cryptic pockets · Water networks · MM/PBSA · GBSA

LAB

Network analysis; compute residue hotspots; inspect water-mediated bridges

Connect structure to mechanism, druggability, and hotspots

DAY 5

Kinetics, Enhanced Sampling & Research Workflows

TOPICS

MSMs · HMMs · Metadynamics · PyEMMA · ML features · TDA · GNN

LAB

Mini kinetic model; bias reweighting; capstone analysis notebook

Complete research-grade pipeline and final presentation

YOUR INSTRUCTORS

20 Years at the Frontier of Molecular Simulation

SC

Dr. Sajeev Chacko

Lead developer of advanced MD analysis techniques

25+ years in computational biophysics. Qunatum Physics, Developed allosteric analysis methods

AS

Dr. Ashutosh Shandilya

Expert in Enhanced sampling & ML-driven MD workflow

Lead developer of pocket detection and bias-reweighting techniques. Expert in kinetics, MSMs, and reproducible pipelines.

SOFTWARE ECOSYSTEM

Tools You'll Master

VISUALIZATION

VMD · ChimeraX

MD ANALYSIS

GROMACS · CPPTRAJ · MDAnalysis

PYTHON & ML

PyEMMA · MDTraj · Scikit-learn

NETWORKS & POCKETS

AADS · fpocket · VolSurf

ENHANCED SAMPLING

aMD · ABPS · GNN reweighting

KINETICS

PyEMMA MSMs · HMMs · TICA

WHAT YOU'LL TAKE HOME

Concrete Deliverables, Every Single Day

Day 1

Clean trajectory movies and publication-ready figure panels

Day 2

Full protein stability report with annotated time-series plots

Day 3

PCA / TICA conformational landscape with clustered states

Day 4

Allosteric network map and druggability assessment

Day 5

Mini kinetic model and bias-reweighted free-energy surface

Repo

Reproducible capstone notebook ready from our GitHub repository

REGISTRATION & RESOURCES

Join the Workshop

All input and output datasets available via our website and GitHub.

Start your analysis on day one — zero setup friction.

Register Now →

DURATION	FORMAT	DATA REPO	CERTIFICATE
5 days · Full day each	Hands-on labs + lectures	GitHub + workshop website	Issued on completion

github.com /BBF-MD-Workshop