Coarse-Grained Models: MARTINI & Elastic Networks — Hands-on

Learn how to use coarse-grained (CG) models to explore slow, large-scale motions of biomolecules using MARTINI and elastic network models. This module covers mapping strategies, CG force fields, elastic networks and normal mode analysis so that you can design multi-scale simulations, interpret low-frequency motions and connect CG insights back to atomistic detail.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Coarse-Graining Concepts & Mapping

Why coarse graining for biomolecules

time and length scale extension **loss of detail vs gain in sampling** **use cases in structural biology**

Mapping atomistic models to coarse-grained sites

bead definitions and mapping rules **proteins, lipids**

and solvent ideas | topology generation workflows

Strengths and limitations of CG models

what observables are meaningful | when atomistic detail is required | designing realistic expectations

Session 2

Fee: Rs 11800 Apply Now

MARTINI Force Field Workflows

MARTINI force field overview

bead types and interaction logic | MARTINI for membranes and proteins | recent developments and variants

Building MARTINI systems from structures

mapping atomistic proteins and lipids | membrane and solvent setup | topology and parameter files

Running and analysing MARTINI simulations

time step and integration settings | common observables for CG simulations | backmapping to atomistic overview

Session 3

Fee: Rs 14800 Apply Now

Elastic Network Models & Normal Modes

Elastic network models (ENMs) for proteins

nodes, springs and contact cutoffs | Gaussian network and anisotropic models | link to crystallographic B factors

Normal mode analysis and low-frequency motions

eigenvalues, eigenvectors, modes | visualising

collective motions | link to conformational transitions

Practical ENM workflows and interpretation

generating ENMs from PDB structures | mode selection and relevance | connecting ENM insights to experiments

Session 4

Fee: Rs 18800 Apply Now

Multi-Scale Modeling & Case Study

End-to-end CG and ENM case study

Theory + Practical

Combining CG MD, ENMs and atomistic views

using ENM modes to guide simulations | backmapping key CG conformations | integrating with docking or FEP plans

Best practices, limitations and reporting

communicating CG assumptions clearly | figures and movies for CG results | methods text and reproducible scripts