

Resolution-Switching in Biomembrane Simulations with Graph Neural Networks

Authors:

Yusuf Eren Tunc, Rainer Böckmann

Molecular dynamics (MD) simulations offer time-resolved, atomistic insight into biomolecular processes, yet conventional, chemically detailed force fields cannot reach the spatial and temporal scales required to study processes such as lipid domain formation or large-scale membrane remodeling. Coarse-grained (CG) approaches like Martini close this gap by representing groups of atoms as single interaction sites (beads), enabling simulations of larger systems over longer times at the expense of chemical resolution. Integrating CG sampling with atomistic-level analysis in a multiscale workflow requires switching between resolutions: reconstructing a chemically detailed configuration from a CG snapshot. This reverse mapping is inherently ill-posed, since a single CG configuration corresponds to an ensemble of possible atomistic structures, and any chosen reconstruction must avoid steric clashes and remain compatible with the target force field.

Here, we introduce a resolution-switching pipeline that uses a graph neural network to reconstruct atomistic lipid bilayers in the CHARMM force field from Martini 3 CG configurations. Each CG configuration is represented as a graph in which beads serve as nodes annotated with chemical and local-environment features, while bonds define edges carrying geometric information. The network predicts the positions of all heavy atoms in a single forward pass. These predicted structures are then completed via automated hydrogen placement, reintroduction of water and ions, and resolution of steric overlaps, followed by standard MD energy minimization, equilibration, and production runs.

We benchmark the method on a range of chemically diverse membrane systems, assessing both local structural fidelity, through bond metrics and coordinate deviations from reference atomistic structures, and collective membrane behavior after re-simulation, including membrane thickness, area-per-lipid distributions, and the leaflet-coupled phase behavior of liquid-ordered versus liquid-disordered domains. Overall, the workflow provides a transferable, end-to-end resolution-switching solution whose reconstructed trajectories recover the structural organization present in the CG ensemble, making it suitable as a general-purpose building block in multi-resolution MD simulation pipelines.