Project topics:

1. Constant pH simulation and an example using Charmm-gui for its implementation using Gromacs.
2. Martini force field (both Martini2 and Martini3) and their comparison using example of protein-only, lipid only and protein-lipid simulation.
3. Alpha fold and Rosetta Fold, RFdiffusion and 2 applications using Charmm-gui.
4. Grand Canonical Monte Carlo simulation and an application using LAMMPS.
5. Replica exchange MD simulation and "REST2" and a demonstration.
6. A comparison of properties and demonstration using simulation of a rigid and flexible water model.
7. Metadynamics simulation versus "OPES simulation" and an example comparison of both of them via simulation using plumed and gromacs.
8. Exploring GENESIS simulation program and a comparison of performance and utility with gromacs using an example
9. "DiffDock" vs "Autodock vina" vs "and an example comparison.
10. QM/MM simulation and an example comparison using Gromacs/CP2K and AMBER/GROMACS.