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Molecular Dynamics Simulations for Beginners: VMD and NAMD

Course Plan

1. Introduction to Molecular Dynamics
   - 1.1 Simulations and their types
   - 1.2 Concept of Molecular Dynamics
   - 1.3 Force Fields
   - 1.4 Numerical Integration and timesteps
   - 1.5 Simulation setup: Ensembles, Periodic Boundary Conditions, Solvation
   - 1.6 Steps of Typical MD simulation
   - 1.7 Conclusions and Applications
2. Modeling and Preparation of Structures: VMD
   - 2.1 Introduction to VMD: download, Basic windows, and loading a pdb file
   - 2.2 Graphics and Coloring in VMD
   - 2.3 Selection and Labeling options in VMD
   - 2.4 Image and Video rendering
   - 2.5 Extensions and Analysis in VMD
   - 2.6 Tk Console Scripting
   - 2.7 Scrips and Plugins
3. Running MD Simulations Using QwikMD/NAMD
   - 3.1 Installing and Preparing NAMD
   - 3.2 Different Files in MD simulation
   - 3.3 Running MD Simulations through *QwikMD* (Explanation)
   - 3.4 Running MD Simulations through *QwikMD* (Practical)
   - 3.5 Resuming or extending a NAMD Simulation
4. Protein-ligand Simulation
   - 4.1 How to get ligand and Protein-ligand structure
   - 4.2 Parametrizing the force field for a ligand
   - 4.3 Running MD simulation for the protein-ligand system in NAMD
5. How to run NAMD on online HPC using *Google Colab* platform
6. Using CHARMM-GUI Server to prepare input files for NAMD
7. Analysis of MD simulations
   - 7.1 How to get your simulation protocol for your publication
   - 7.2 Analysis of MD Simulations using *QwikMD* plugin
   - 7.3 Analysis of MD Simulations using VMD and Analysis Scripts
   - 7.4 Analysis of MD Simulations using External packages: MDTraj, Bio3D, and Others
8. Introduction to Binding Free Energy Calculation
   - 8.1 Free Energy Calculations: Theoretical Introduction
   - 8.2 Relative Binding Free Energy Calculations: MMGBSA
   - 8.3 Absolute Binding Free Energy Calculations: BFEE

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Molecular Dynamics Simulations for Beginners

Course Schedule: 3 Hours each day, 6 sessions. All the times are in Jordan, Amman time, PM. (You can see your timezone by searching: 3 PM Jordan time to ------)

Date	Day	Time	Tittle	Notes
26/2/2022	Saturdy	3:00-3:20	Intro and Welcome	----------
		3:20-4:20	Introduction to Molecular Dynamics Simulations of Proteins and Biomolecules	Theoretical lecture about the basics of MD Simulations
		4:40-6:00	Introduction to Molecular Dynamics Simulations of Proteins and Biomolecules – continued	Theoretical lecture about the basics of MD Simulations

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Date	Day	Time	Tittle	Notes
27/2/202	Sunday	3:00-4:00	Visual Molecular Dynamics (VMD)	Hands-on session on using VMD software for visualization and static analysis
		4:00-4:20	Break	----------
		4:20-6:00	Visual Molecular Dynamics (VMD)	Hands on session on using VMD software for visualization and static analysis

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Date	Day	Time	Tittle	Notes
28/2/2021	Monday	3:00-4:10	Running Molecular Dynamics Simulation on NAMD using QwikMD plugin	How to carry MD simulations easily using QwikMD in VMD software
		4:30-5:00	Different types of files in MD Simulations, Editing the input files	PDB, PSF, TOPOLGY, PARAMETER, CONFIG Files explained
		5:00-6:00	Protein – ligand MD simulation, force-field parametrization for a ligand, running and preparing protein-ligand MD simulation on NAMD	Protein-ligand system

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Date	Day	Time	Tittle	Notes
1/3/2022	Tuesday	3:00-3:45	How to run NAMD molecular dynamics simulation on free HPC resources using google colab platform	How to run NAMD simulations using online free GPU resources
		3:45-4:30	Using CHARMM-GUI to prepare NAMD	CHARMM-GUI Server
		4:45-6:00	How to resume or extend a NAMD simulation	

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Date	Day	Time	Tittle	Notes
2/3//2022	Wednesday	3:00-3:30	Analysis of MD Simulations: Protocol and Quality Check	How to get your MD protocol
		3:30-4:30	Analysis of MD Simulations: Protein System	RMSD, RMSF, ENERGIES, H-BONDING, SALT-BRIDGES, SASA, AND OTHER VALUES
		4:50-6:00	Analysis of MD Simulations: Protein-ligand Systems	RMSD, RMSF, H-BONDING, SALT-BRIDGES, ROG, SASA, CONTACT AREA, CONTACT FREQUENCY

Date	Day	Time	Tittle	Notes
3/3/2022	Thursday	3:00-3:40	Introduction to Binding Free Energy Calculations	----------
		3:40-4:40	Relative Binding Free Energy Calculations for NAMD output: MMGBSA Calculation	
		5:00-6:00	Absolute Binding Free Energy Calculations for NAMD output: BFEE Plugin	

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