Schedule (FunMolSim - 2019)

Date & Day	Time	Session	Speaker	Topic
March 5, Day 1	8.30-9.00 am	Registration		
	9.00-10.30 am	Lecture	Jayant Singh	Introduction to Molecular Simulations, Ensembles and Connection to Thermodynamics
	10.30-11.00 am	Tea Break		
	11.00-12.30 pm	Lecture/Tutorial	Jayant Singh	Computing Interaction Potential Forces
	Lunch Break			
	2.00-3.30 pm	Lecture	Pankaj Apte	Basics of Molecular Dynamics Simulation
	3.30–4.00 pm	Tea Break		
	4.00-5.30 pm		Pankaj Apte	Molecular Dynamics Simulations
March 6, Day 2	9.00-10.30 am	Lecture	Ganapathy Ayappa	Extended Systems Molecular Dynamics, NVT, NPT
	10.30-11.00 am	Tea Break		
	11.00-12.30 pm	Tutorial	Ganapathy Ayappa	Tutorial on extended systems MD
	Lunch Break			
	2.00-5.00 pm	Lab session	Sandip Khan	Hands on MD s/w –LAMMPS, GROMACS

March 7, Day 3	9.00-10.30 am	Lecture	Jayant Singh	Monte Carlo Simulations: Importance Sampling – Metropolis Method
	10.30-11.00 am	Tea Break		
	11.00-12.30 pm	Tutorial/Lab Session	Jayant Singh/Sandip Khan	Hands on Monte Carlo Simulation code-
	Lunch Break			
	2.00- 3.30 pm	Lecture	Jayant Singh/Sandip Khan	Monte Carlo in other Ensembles (NPT, GCMC)
	3.30-4.00 pm	Tea Break		
	4.00-5.30 pm	Tutorial	Jayant Singh/Sandip Khan	Monte Carlo in different ensemble- case studies- Adsorption isotherm estimation
March 8, Day 4	9.00-10.30 am	Lecture	Jhumpa Adhikari	Phase equilibria Calculations using molecular simulations
	10.30-11.00 am	Tea Break		
	11.00-12.30 pm	Tutorial	Jhumpa Adhikari	Tutorial: Phase diagram calculations via MC methods
	Lunch Break			
	2.00-3.30 pm	Lecture	Jayant Singh	Free-energy methods (Parallel tempering, Umbrella sampling, Meta dynamics)

	3.30-4.00 pm	Tea Break		
	4.00-5.30 pm	Tutorial	Jayant Singh	Calculating free-energy: cases studies
	7.30 pm	Course Dinner		
March 9, Day 5	9.00-10.30 am	Lecture	Ethaya Mani	Soft Matter Simulations-Monte Carlo and Kinetic Monte Carlo, Coarse-grain approaches
	10.30-11.00 am	Tea Break		
	11.00-12.30 pm	Tutorial	Ethaya Mani	Hands on KMC simulations of Soft Matter
	Lunch Break			
	2.00-3.30 pm	Lecture	Indranil Saha Dalal	DPD/Brownian Simulations
	3.30-4.00 pm	Tea Break		
	4.00-5.30 pm	Tutorial	Indranil Saha Dalal	Hands on DPD and Brownian simulations