

Date	Session	Chaired by	Time (CET) [PST]	CT / Keynote / discussion	Speaker	Title of the talk
11 December	Session 1	Rebecca Wade	(5pm) [8am]	Welcome		
			(5:10pm) [8:10am]	Keynote talk 1	Adrian Elcock	Brownian dynamics simulations of large biomolecular systems with hydrodynamic interactions
			(5:50pm) [8:50am]	CT1	Hender Lopez	Machine Learning approach to include Hydrodynamics interactions in Brownian Dynamics simulations
			(6:10pm) [09:10am]	Keynote talk 2	Johannes Schoeneberg	
	break		(6:50pm) [09:50am]	break	break	break
	Session 2	Riccardo Beccaria	(7:15pm) [10:15am]	Keynote talk 3	Maciej Dlugosz	Accurate Estimation of Diffusion Coefficients of Confined Molecules with Shape-Based Coarse-Graining and Mobility Scaling.
			(7:55pm) [10:55am]	CT2	Debabrata Dey	Lost in the Cytoplasm: A Journey of Weakly Basic Drugs Through Cellular Crowding
(8:15pm) [11:15am]			Discussion/Software updates		Software Updates Overview	
end of day 1		(9pm) [12:00pm]	end of day 1	end of day 1	end of day 1	
12 December	Session 3	Chia-en Chang	(5pm) [8am]	Welcome		
			(5:05pm) [8:05am]	Keynote talk 4	Tamar Schlick	Folding genomes at nucleosome resolution
			(5:45pm) [8:45am]	CT3	Parisa Fasihianifard	Molecular Encounter Efficiency in Cellular Environments: Brownian Dynamics Insights into Molecular Binding
			(6:05pm) [09:05am]	CT4	Riccardo Beccaria	Protein-Ligand Association in Crowded Media: a Multiscale Brownian Dynamics Simulation Approach
			(6:25pm) [09:25am]	Discussion/Software updates		Discussion and Q&A on Updates
	break		(7pm) [10am]	break	break	break
	Session 4	Rommie Amaro	(7:15pm) [10:15am]	Keynote talk 5	Sarah Harris	Multi-meso: Mesoscale modelling of Molecular Machines and MesoSoup
			(7:55pm) [10:55am]	CT5	Abraham Muniz Chicarro	Multiscale approach to predict drug-protein binding kinetics
			(8:15pm) [11:15am]	CT6	Lane Votapka	Multiscale Simulation Approaches To Computational Binding Kinetics with SEEKR
			(8:35pm) [11:35am]	Discussion/Software updates		What's next?
end of day 2		(9pm) [12:00pm]	end of day 2	end of day 2	end of day 2	