CECAM Flagship School: Systematic coarse-graining and machine learning in soft matter physics with ESPResSo

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00	Lecture: Introduction to particle-based simulations, R. Weeber	Lecture: Introduction to machine learning, K. Nikolaou	Lecture: Chemical space exploration and reverse CG, T. Bereau	Lecture: TBA, C. Junghans	Scientific talk: TBA, N. van der Vegt
10:00	Lecture: ESPResSo applications, J.-N. Grad			Scientific talk: TBA, M. Miettinen	Scientific talk: TBA, J. Zavadlav
	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:00	Lecture: Introduction to systematic coarse-graining, D. Andrienko	Lecture: Machine Learning descriptors, P. Loche	Lecture: Soft matter, A. Schlaich, C. Holm	Lecture: Lattice-Boltzmann hydrodynamics and active matter, R. Weeber	Scientific talk: TBA, S. Tovey
12:00					Scientific talk: TBA, S. Olsson
13:00	Lunch break	Lunch break	Lunch break	Lunch break	Concluding remarks
					Lunch break
14:00	Hands-on session: Lennard-Jones fluid	Hands-on session: ML potential for water, comparison to atomistic water model, part 1	Hands-on session: Chemical space exploration (and/or reverse CG)	Hands-on session: Polymers diffusion	
15:00					
	Coffee break	Coffee break	Coffee break	Coffee break	
16:00	Hands-on session: Boltzmann inversion	Hands-on session: ML potential for water, comparison to atomistic water model, part 2	Hands-on session: TBA	Hands-on session: Active matter with reinforcement learning	
17:00					
18:00	Social event & barbecue	Poster session & aperitif		City tour and conference dinner	
19:00					
20:00					