

Simulating the dynamics of soft matter with ESPResSo, PyStencils and LbmPy

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00	Lecture: Introduction to particle-based simulations	Lecture: Charged matter	Lecture: WaLBerla: <u>Overview and examples</u>	Lecture: Active matter	Lecture: Lees-Edwards for shear flow, polymers
10:00	Lecture: ESPResSo applications	Lecture: Polymers	Lecture: Introduction to <u>SymPy with live demo</u>		
	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:00	Lecture: Electrostatics solvers	Lecture: Lattice-Boltzmann	Hands-on session: Diffusion advection equation using PyStencils	Lecture: Electrokinetics	Scientific talk
12:00	Lecture: Error analysis			Lecture: Data management with git, pandas, MDSuite	Scientific talk
					Concluding remarks
13:00	Lunch break	Lunch break	Lunch break	Lunch break	Lunch break
14:00	Hands-on session: Lennard-Jones fluid	Hands-on session: Lattice-Boltzmann (part 1)	Lecture: Automated code generation with LbmPy	Hands-on session: Active matter	
15:00	Coffee break	Coffee break	Coffee break		Coffee break
16:00	Hands-on session: Charged matter	Hands-on session: Lattice-Boltzmann (part 2)	Hands-on session: Two-component fluid simulations with Shan-Chen	Scientific talk or dev meeting	
17:00	Social event (onsite participants)	Scientific talk	Scientific talk	City walk and speaker's dinner (onsite participants)	

Schedule for the CECAM Flagship School ESPResSo, October 10–14, 2022, Central European Summer Time (UTC+02).