

Simulating energy materials with ESPResSo and waLBerla

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00	Lecture: Introduction to particle-based simulations, R. Weeber	Lecture: Electrostatics in confinement, C. Holm, A. Schlaich	Lecture: Lattice-Boltzmann method, S. Gekle	Lecture: Reaction methods, P. Košován	Scientific talk
10:00	Lecture: ESPResSo applications, C. Lohrmann				Scientific talk
	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:00	Lecture: Data management, R. Weeber	Lecture: Supercapacitors and batteries, M. Salanne	Lecture: Two-phase LB methods, A. Reinauer	Lecture: Catalysis and reactive forcefields, T. Jacob	Scientific talk
12:00	Lecture: Error analysis, J.-N. Grad		Lecture: Electrokinetic methods, C. Lohrmann		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: Electrostatics in confined systems (part 1)	Hands-on session: LB sedimentation	Hands-on session: Chemical reactions	Note The school ends on Friday at 1pm. The lecture blocks may be swapped in the final schedule.
15:00	Coffee break	Coffee break	Coffee break	Coffee break	
16:00	Hands-on session: Error analysis	Hands-on session: Electrostatics in confined systems (part 2)	Hands-on session: Electrokinetics in flow	Community meeting	
17:00	Social event (onsite participants)	Poster session (onsite participants)		City walk and speaker's dinner (onsite participants)	

Preliminary schedule for the CECAM Flagship School ESPResSo, October 9–13, 2023, Central European Summer Time (UTC+02).