

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: The lattice-Boltzmann method, S. Gekle	Lecture: Reaction methods, P. Košovan	Scientific talk: Ion dynamics in conductive nanopores, S. Kondrat
10:00	Lecture: ESPResSo applications, C. Lohrmann				Scientific talk: ML potentials, S. Tovey
	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:00	Lecture: Data management, R. Weeber	Lecture: Challenges in the modeling of energy storage devices, M. Salanne	Lecture: Two-phase LB methods, A. Reinauer	Lecture: Catalysis and reactive forcefields, T. Jacob	Scientific talk: Metallic interfaces, L. Salfi
12:00	Lecture: Error estimation in time-correlated data, J.-N. Grad		Lecture: Electrokinetic methods, C. Lohrmann		Scientific talk: Ferrofluids and ferrogels, R. Weeber
					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 of ion condensation	Hands-on session: LB sedimentation	Hands-on session: The constant pH method	
15:00	Coffee break	Coffee break	Coffee break	Coffee break	
16:00	Hands-on session: Error analysis	Hands-on session: Electrolytic capacitors	Hands-on session: Electrokinetics in flow	Community meeting	
17:00	Poster session and social event (onsite participants)	Scientific talk: Multiscale models for energy materials, C. Merlet		City walk and speaker's dinner (onsite participants)	

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