

Summer School – Computational Methods

25-27/09/2025

Thursday 25th of September 2025

Multi-scale Modeling / Atomistic & DPD Simulations of Soft Matter	
Time EET	Topics
09:00 – 10:30	Anastassia Rissanou, Vagelis Harmandaris - Computational Modeling of Soft Matter Across Scales
10:30 – 11:00	Coffee Break
11:00 – 12:30	Anastassia Rissanou – Hands-on Session on Molecular Simulations of Biomolecules
12:30 – 14:00	Lunch
14:00 – 15:30	Safa Jamali – Modeling of Soft Matter using Dissipative Particle Dynamics
15:30 – 16:00	Coffee Break
16:00 – 17:30	Safa Jamali – Hands-on Session on Dissipative Particle Dynamics for Colloidal Systems



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Contacts

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Zoom link:

<https://us02web.zoom.us/j/83567821942?pwd=8UiiLeSNMwHT6U3pNTieRiTXVI5wsD.1>

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Friday 26th of September 2025

Mesoscopic Modeling of Soft Matter	
Time EET	Topics
09:00 – 10:30	Marisol Ripoll, Tyler Shendruk– Multi-particle Collision Dynamics
10:30 – 11:00	Coffee Break
11:00 – 12:30	Marisol Ripoll, Tyler Shendruk - Hands-on Simulations using Multi-particle Collision Dynamics (MCDP) approach
12:30 – 14:00	Lunch
14:00 – 15:30	Roseanna Zia (online) – Stokesian Dynamic
15:30 – 16:00	Coffee Break
16:00 – 17:30	Joost de Graaf – Hands-on Session on Simulations using Stokesian Dynamics

Saturday 27th of September 2025

Data-driven Modeling and Machine Learning in Soft Matter	
Time EET	Topics
09:00 – 10:30	Oleksandra Kukharenko – Introduction to AI/ML Methods in Material Science
10:30 – 11:00	Coffee Break
11:00 – 12:30	Oleksandra Kukharenko – Introduction to AI/ML Methods in Material Science
20:00	Social dinner