Week 1

M3-FSC2SB: Multiscale Modelling Methods 2025

The schedule is subject to change. Times are for guidance only.

Monday, July 14th

09:00–09:20	Welcome at MUNI
09:20–09:40	Computational Cluster Accounts
09:40–10:00	Survive Brno
10:20–10:35	WOLF Cluster
10:35–10:50	Coffee Break
10:50–11:05	Survey
11:05–11:15	School Scope
11:15–12:15	Introduction to Molecular Modelling 1
12:15–13:15	Lunch
13:15–14:10	Introduction to Molecular Modelling 2
14:10–15:00	SCM: Selected Applications of Computational Chemistry for Materials Modelling

Tuesday, July 15th

09:00–09:50	Linux
09:50–10:20	Potential Energy Surface, Structure Visualization
10:20–10:40	3D Printing in Molecular Modelling
10:40–10:55	Coffee Break
10:55–12:00	Quantum Mechanics
12:00–13:00	Lunch
13:00–14:15	Supramolecular Systems
14:15–15:00	Conformational Search

Wednesday, July 16th

09:00–09:10	Summary/Revision
09:10–10:30	Studying Reactions using PES-Based Methods 1
10:30–10:45	Coffee Break
10:45–12:00	Studying Reactions using PES-Based Methods 2
12:00–13:00	Lunch
13:00–13:30	Molecular Mechanics
13:30–14:00	Molecular Dynamics 1
14:00–15:00	Unbiased Molecular Dynamics in AMBER
15:00–16:00	NMR Core Facility Excursion (Optional)

Thursday, July 17th

09:00–09:45	Molecular Dynamics 2
09:40–10:30	Molecular Dynamics 3
10:30–10:45	Coffee Break
10:45–12:00	ReaxFF Simulations
12:00–13:00	Lunch
13:00–14:15	Free Energy Calculations 1
14:15–15:00	Biased Molecular Dynamics in AMBER
16:00–22:00	Get-together Meeting & Dinner

Friday, July 18th

09:00–09:10	Summary/Revision
09:10–10:40	Nucleic Acid Simulations 1
10:40–10:55	Coffee break
10:55–12:20	Nucleic Acid Simulations 2
12:20–12:30	Survey
12:30–13:30	Lunch
13:20–15:00	General Discussion

Week 2

M3-FSC2SB: Multiscale Modelling Methods 2025

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Monday, July 21st

09:00–09:40	Why Simulations? Biomolecular Overview
09:40–10:00	Intro to GROMACS and Jupyter Notebooks
10:00–10:15	Coffee Break
10:15–12:00	Intro to GROMACS and Jupyter Notebooks
12:00–13:00	Lunch
13:00–14:00	Biosimulations with CHARMM-GUI Part 1
14:00–15:00	Biosimulations with CHARMM-GUI Part 2

Tuesday, July 22nd

09:00–09:55	Protein Coarse-Graining
09:55–10:10	Coffee Break
10:10–11:10	Protein Coarse-Graining
11:10–12:00	Free Energy Calculations - GROMACS & PLUMED
12:00–13:00	Lunch
13:00–15:00	Free Energy Calculations - GROMACS & PLUMED
15:00–16:00	CryoEM Core Facility Excursion (Optional)

Wednesday, July 23rd

09:00–09:20	Summary/Revision
09:20–10:25	Supercomputing
10:25–10:40	Coffee Break
10:40–11:20	X-ray Structure Determination
11:20–12:00	CryoEM Structure Determination
12:00–13:00	Lunch
13:00–14:00	AI in Structural Biology
14:00–15:00	Structure Prediction
15:00–16:00	IT Museum + CEITEC Server Room (Optional)

Thursday, July 24th

09:00–10:00	Structure Prediction
10:00–11:00	Docking
11:00–11:15	Coffee break
11:15–11:45	QM/MM Simulations 1
11:45–12:15	Free Energy Simulations 2
12:15–13:15	Lunch
13:15–14:30	QM/MM Simulations 2
14:30–15:00	Free Energy Simulations 3

Friday, July 25th

09:00–10:30	QM/MM Simulations 3
10:30–10:45	Coffee break
10:45–11:45	Summary/Revision
11:45–12:00	Survey
12:00–13:00	Lunch
13:00–15:00	Open Discussion

Notes:
The computer cluster (room) availability:

- the local access during the summer school from 9:00 to 19:00 on working days
- the remote access from the web browser till September 7th

Consultations of optional exercises upon prior request during the summer school from 15:00 to 18:00 on working days

Summer School Web:
https://www.ncbr.muni.cz/en/for-students/summer-schools/2025/m3-fsc2sb