

International Spring School Statistical Thermodynamics 2017

Time	Mon. 20/11/17	Tue. 21/11/17	Wed. 22/11/17	Thur. 23/11/17	Fri. 24/11/17	Mon. 27/11/17	Tue. 28/11/17	Wed. 29/11/17	Thur. 30/11/17	Fri. 01/12/17	
9:00	Free Time	Welcome JAG	Free Time	Free Time	Free Time	Free Time	Free Time	Free Time	Free Time	Free Time	
9:30		Lecture 1: Overview and Introduction JAG	Lecture 4: Thermodynamics JAG	Lecture 7: Classical Mechanics I JAG	Lecture 10: Ensembles I CO	Lecture 13: Free energies: reaction coordinates JAG	Lecture 16: Calculating properties from simulations JAG	Lecture 19: Electrostatics WvG	Lecture 22: On the ethics of the academic endeavour: where do we go? WvG	Lecture 24: Left-overs/ questions and future perspectives WvG	
10:15		Break	Break	Break	Break	Break	Break	Break		Break	
10:30		Lecture 2: Molecular Simulations MD/SD/MC CO	Lecture 5: Force-Field Development CO	Lecture 8: Classical Mechanics II JAG	Lecture 11: Ensembles II JAG	Lecture 14: Boundary Conditions I WvG	Lecture 17: Comparison with Experiments WvG	Lecture 20: Polarization WvG	Lecture 25: Students plans I WvG		
11:15		Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break		
11:45		Lecture 3: How to simulate using GROMOS CO	Lecture 6: Structure Refinement CO	Lecture 9: Analyzing with GROMOS CO	Lecture 12: Free energies: alchemy CO	Lecture 15: Boundary Conditions II WvG	Lecture 18: Searching & Enhanced Sampling WvG	Lecture 21: Multi-resolution simulations WvG	Lecture 23: QM/MM WvG	Lecture 26: Students plans II	
12:30		Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Break for lunch, self-study, discussion.*	Tutorial 10: **	
14:00		Registration	Tutorial 2: Running MD GROMOS Tutorial	Tutorial 3: Running MD Students Plans	Tutorial 4: Running MD Students Plans	Tutorial 5: Running MD Students Plans	Tutorial 6: Statistical Mechanics exercises	Tutorial 7: Analyzing MD: GROMOS Tutorial	Tutorial 8: Analyzing MD: Students Plans	Tutorial 9: Analyzing MD: Students Plans	How to prepare a barbecue
16:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	
17:30		End of session	End of session	End of session	End of session	End of session	End of session	End of session	End of session	End of session	
20:30	Free time	Free time	Free time	Free time	Free time	Free time	Free time	Free time	Free time	Farewell	

CO: Chris Oostenbrink, WvG: Wilfred van Gasteren, JAG: José Antonio Gárate

*Campus restaurant, Parque Tecnológico Zañartu

**Football field, Parque Tecnológico Zañartu

Lectures venue: Central Auditorium, 4th floor, Fundación Ciencia & Vida