

Seminar WS12/13: Computersimulationen von weicher Materie - Grundlagen und ausgewählte Methoden

Topic (Mentor/Speaker) *Basics

- 1.* **25.10.2012** - Examples and stat. Mech. (Dzubiella)
- 2.* **01.11.2012** - Molecular Dynamics Simulations; Hamiltonian; Newton; leap-frog algorithm, Ensembles NVT and NPT, Thermostats and Barostats (Gregor Weiss)
- 3.* **08.11.2012** - Brownian dynamics (Heptner); Ermak and McCammon algorithm, Hydrodynamic approximation via Oseen Tensor
- 4.* **15.11.2012** - Monte Carlo Simulations (Dzubiella); grand canonical simulations, Markov processes, detailed balance, Metropolis, smart moves
- 5.* **22.11.2012** - Ewald summation (Yigit); periodic boundary conditions, particle mesh ewald, derivation and implementation
- 6.* **29.11.2012** - Free energy calculations (Palczynski); thermodynamic integration, test particle insertion, free energy perturbation, umbrella sampling
- 7.* **06.12.2012** - Replica exchange Methods (Heyda)
8. **13.12.2012** -Dissipative Particle Dynamics (DPD) and related Methods (Heptner)
9. **20.12.2012** -Rare events I (Heyda, Palczynski); Bennett-Chandler, Transition path sampling, string method
10. **10.01.2013** - Rare events II (Palczynski, Heyda); forward flux sampling
11. **17.01.2013** - Protein simulations I (Yigit/Dzubiella); Simulation packages; water models, amino acids, force fields;
12. **24.01.2013** - Protein simulations II (Yigit/Dzubiella); visualization, tools, analysis
13. **31.01.2013** - Hardware, parallelization, GPU computing (Dzubiella, Heptner)??
14. **07.02.2013??**
15. **14.02.2013??**