Biomolecular modeling

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Exam topics

1. Total energy with molecular mechanics
   - bonded and non-bonded interactions
   - contributions to the energy
   - parameters and variables in the energy contributions
   - relation of force and energy
2. Molecular dynamics simulation
   - equations of motion
   - their numerical solution
   - initial conditions
   - Verlet method
   - time step
   - conservation of energy

Exam topics

3. Temperature and MD simulation
   - relation of temperature
   - kinetic energy and velocities
   - scaling of velocities to control temperature
   - Berendsen thermostat
4. Setup of molecular system to be simulated
   - periodic boundary conditions
   - shape of the box
   - MM models of water
   - treatment of non-bonded interactions (cut-off, Ewald method)

Exam topics

5. Analysis of simulation
   - average structure
   - RMSD
   - RMSF
   - radial distribution function
6. Coarse-grained simulations
   – in the extent of the slide deck from the class
7. Enhanced sampling methods
   - statement of the problem
   - metadynamics
     - principle
     - application of additional energy contribution
     - need of a collective variable
     - free energy as function of CV