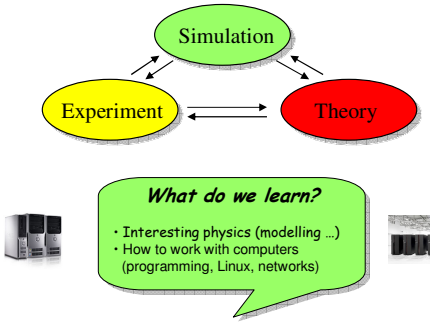
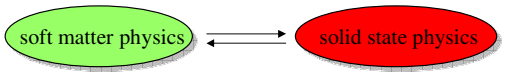
Computer Simulations in Statistical Physics



Computer Simulations in Statistical Physics

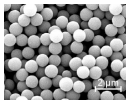


Dr. Peter Virnau

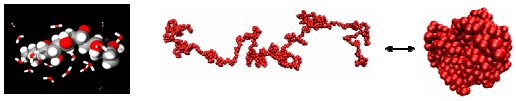
Prof. Nils Blümer

Typical soft matter systems?

Polymers, Proteins, DNA, Lipids, Colloids, …

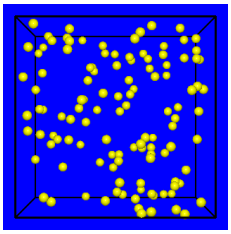


Oligomers / Polymers



Biopolymers: Proteins, DNA, Membranes

Classical molecular simulation – How does it work?



Starting point:

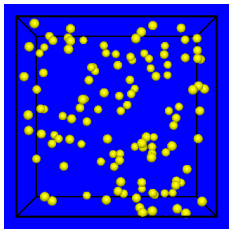
e.g. cubic simulation box filled with particles

Goal: Determine equilibrium properties (e.g. typical distance between particles)
or dynamical properties of the system

How?: Generate many statistically independent configurations and "measure" quantities
Molecular Dynamics / Monte-Carlo

Determine equilibrium properties by averaging over all configurations
Analyze evolution of systems with time (dynamics)

Statistical ensembles:



Example:

Canonical (N,V,T) ensemble
i.e., particle number, volume and temperature are fixed
→ pressure fluctuates

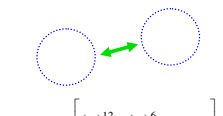
(N,P,T)-ensemble
i.e. particle number, pressure and temperature are fixed
→ volume of the simulation box fluctuates

Grandcanonical (μ,V,T) ensemble
i.e., chemical potential, volume, and temperature are fixed
→ Particle number in the box fluctuates (insert/delete particles)

How do we describe molecules in (classical) simulations?

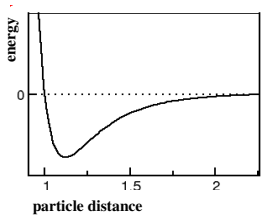
"via force-fields" (expression for the energetic interactions between two particles)

Example: The Lennard-Jones potential (noble gases)



$$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \underbrace{\frac{127}{16384}}_{\Delta U_{cut\ off}}\right]$$

$$r_{cut\ off} = 2\sqrt[6]{2}\sigma$$



Simulation techniques: Molecular Dynamics

Idea: "Solve Newton's equation of motion"

$$\vec{F} = m\vec{a} = m\dot{\vec{v}} = -\nabla U$$

"Recipe":

Starting configuration, "force field" (potential)

In each time step:

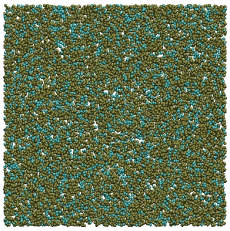
|: Determine forces between all particles

→ move particles :|

Simulation techniques: Molecular Dynamics

Idea: "Solve Newton's equation of motion"

Example: Demixing of polymer solution

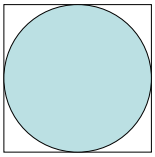


Dr. Leonid Yelash

Simulation technique: Monte Carlo

Idea: "Solve problems by drawing random numbers"

Example: Determine Pi:



$$\Pi = \frac{4A_{\circ}}{A_{\square}}$$

Implementierung:
http://www.eveandersson.com/pi/monte-carlo-circle

Simulation technique: Monte Carlo

Idea: "Solve problems by drawing random numbers"

Recipe: Metropolis algorithm

Starting configuration, "force field" (potential)

|: Modify existing configuration (e.g. move a particle)

Determine the energy difference between two particles

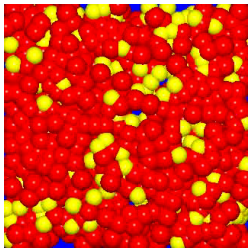
Energy lower? → accept new configuration

Energy higher? → accept with probability exp(-1/kT ΔE) :|

Simulation technique: Monte Carlo

Idea: "Solve problems by drawing random numbers"

Example: Nucleation



Time and length scales in simulation