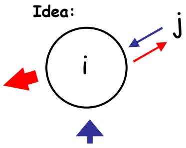
Recap: Importance sampling

Idea:



Master Equation:

Equilibrium:

„ Flow out of state i = Flow into state i"

$$\sum_{j \neq i} P_i(t) W_{i \to j} = \sum_{j \neq i} P_j(t) W_{j \to i}$$

P is Boltzmann-distributed:

$$P_i(t) = \frac{1}{Z_{kan}} e^{-\beta E_i}$$

Detailed Balance:

$$P_i(t) W_{i \to j} = P_j(t) W_{j \to i}$$

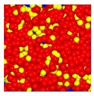
Metropolis Criterion:

$W_{i \to j} = 1$, if $\Delta E = (E_j - E_i) < 0$

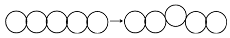
$W_{i \to j} = \exp(-\beta \Delta E)$, if $\Delta E > 0$

„Numerical Recipe": Local Displacements

Starting configuration



|: Move a particle



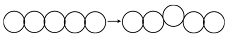
Determine the energy difference between old and new configuration

Energy lower? → Accept the move

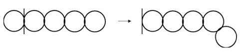
Energy higher? → Accept with probability $\exp(-1/kT\ \Delta E)$

[Draw random number 0<r<1 :
r < $\exp(-1/kT\ \Delta E)$ → accept
else → reject move] :|

Canonical polymer MC moves

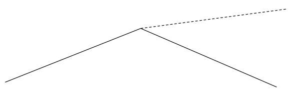


Local Displacement



Slithering Snake

Pivot



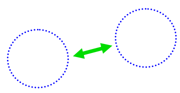
Not considered:
Chain-growth algorithms:

Configurational Bias, Recoil Growth, PERM
...

How do we define energy in our system?

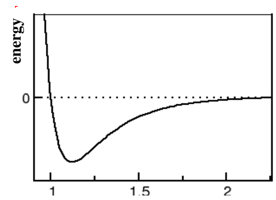
Def. **force-field:** Expression for the energetic interactions between two particles

Example 1: The Lennard-Jones potential (noble gases)



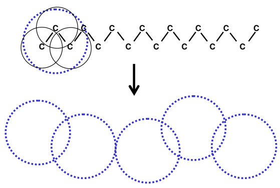
$$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \underbrace{\frac{127}{16384}}_{\Delta U_{cut\ off}}\right]$$

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



How do we define energy in our system?

Example 2: Coarse-grained polymer models

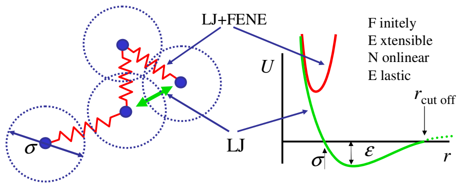


$C_{16}H_{34}$ – chain of 5 monomers

Bead-Spring-Model

How do we define energy in our system?

Example 2: Coarse-grained polymer models (bead-spring model)



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

$$U_{FENE}(r) = -33.75 \ln\left(1 - \left(\frac{r}{1.5\sigma}\right)^2\right)$$

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