Various topics

Grand canonical Monte Carlo

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Grand canonical Monte Carlo simulation

grand canonical ensemble: μVT

(compare with canonical ensemble: NVT)

constant chemical potential, variable number of particles

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GCMC

- explicitly accounts for density fluctuations
  at fixed volume and temperature
- trial insertions and deletions of molecules

Grand canonical Monte Carlo simulation

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calculation of the acceptance probability:

$$\mathcal{P}(N \to N+1) = \frac{V\Lambda^{-3}}{N+1} \cdot \exp[\beta\mu] \cdot \exp[-\beta(U_{N+1} - U_N)]$$

$$\mathcal{P}(N \to N-1) = \frac{N}{V\Lambda^{-3}} \cdot \exp[-\beta\mu] \cdot \exp[-\beta(U_{N-1} - U_N)]$$

($\beta = \frac{1}{k_B T}$, de Broglie thermal wavelength $\Lambda = \sqrt{\frac{h^2}{2\pi m k_B T}}$)

note: practical implementations differ a little

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- interfaces – e.g. studies of adsorption
- protonation states of amino acid side chains in a protein
  – chemical potential of protons is related to pH
- water molecules in a binding pocket / another cavity
  – work with the chemical potential of water