# MCMD model. Grand reaction ensemble

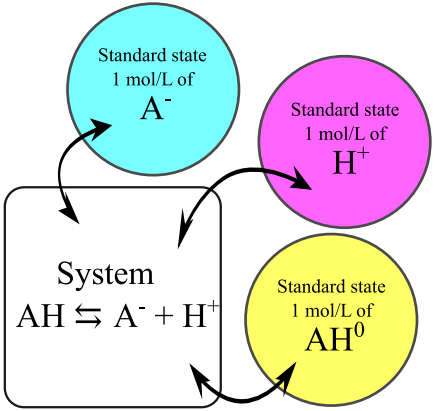
System free energy

$$\Omega = E - TS + \sum_i \left(\mu_i - \mu_i^{\ominus}\right) N_i$$

Reactions

$$\mathrm{HA} \overset{K}{\leftrightarrows} \mathrm{A^-} + \mathrm{H^+} \qquad K = \mu^{\ominus}_{\mathrm{H^+}} + \mu^{\ominus}_{\mathrm{A^-}} - \mu^{\ominus}_{\mathrm{HA}}$$

$$\emptyset \leftrightarrows \mathrm{Na^+} + \mathrm{Cl^-} \qquad K = \mu_{\mathrm{Na^+}} + \mu_{\mathrm{Cl^-}}$$




The change of system free energy during a reaction step

$$\Delta\Omega = k_B T \ln\left(\prod_i V^{\nu_i \xi} \frac{N_i!}{(N_i + \nu_i \xi)!}\right) + \xi\left(\sum_i \nu_i \mu_i - \sum_i \nu_i \mu_i^{\ominus}\right) + \Delta E$$

$$\boxed{\Delta\Omega = k_B T \ln\left(K^{\xi} \prod_i V^{\nu_i \xi} \frac{N_i!}{(N_i + \nu_i \xi)!}\right) + \Delta E}$$

accept if $\mathcal{R}^{\xi} < e^{\Delta\Omega / k_B T}$