Introduction to Bioinformatics

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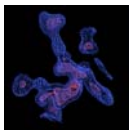
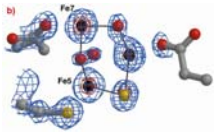
Protein Modeling Methods

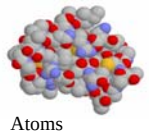
- ***Ab initio* methods:**
  solution of a protein folding problem
  search in conformational space
- **Energy-based methods:**
  energy minimization
  molecular simulation
- **Knowledge-based methods:**
  homology modeling
  fold recogniion

Molecular structure representation

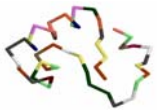




Elementary particles



Atoms



Groups of atoms

Potential Energy Function

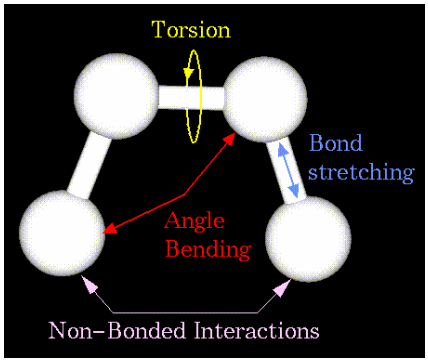
$$PEF(R) = \sum_{bonds} K_b\{b(R)-b_{eq}\}^2 + \sum_{angles} K_\theta\{\theta(R)-\theta_{eq}\}^2 +$$

$$\sum_{dihedrals} \frac{K_\phi}{2}\{1 + \cos[n\phi(R) - \gamma]\} +$$

$$\sum_{\substack{non\text{-}bonded\\ atom\ pairs\ i,j}} \left[\frac{A_{ij}}{r_{ij}(R)^{12}} - \frac{B_{ij}}{r_{ij}(R)^{6}} + \frac{q_i q_j}{\varepsilon_r \varepsilon_0 r_{ij}(R)} \right] \quad (1)$$

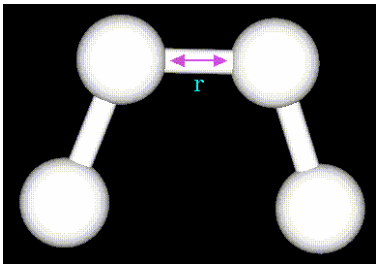
Forcefields: AMBER, CHARMM, CVF, ECEPP, GROMOS

Non-Bonded Interactions

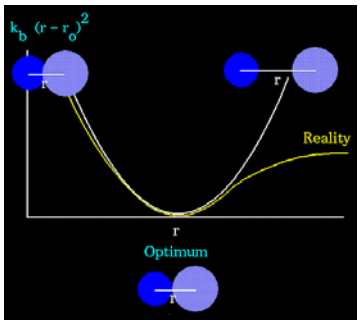


Bond length

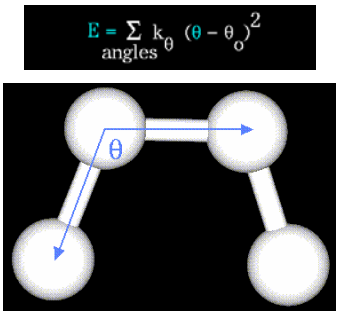
$$E = \sum_{bonds} k_b (r - r_o)^2$$



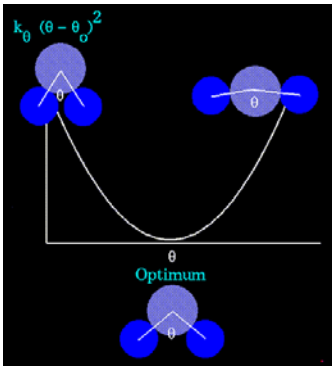
Bond length



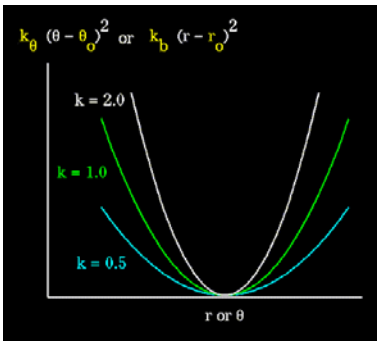
Bond angle



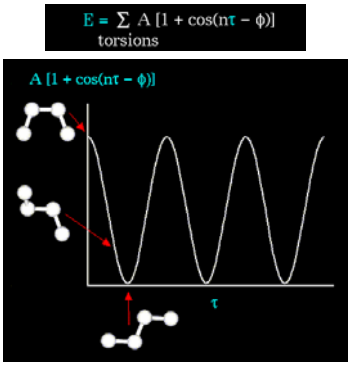
Bond angle



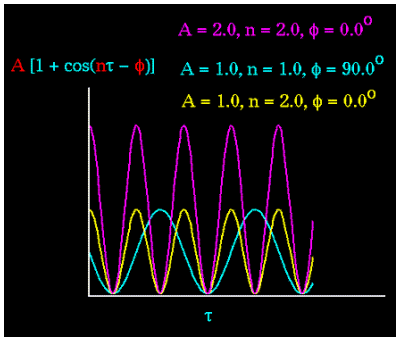
Bond length and angle (parameters)



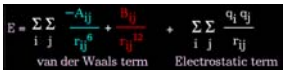
Torsional angle

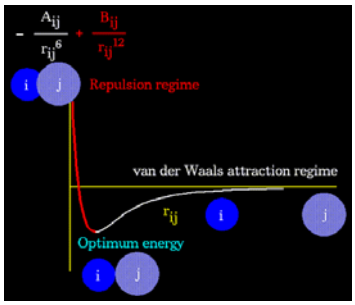


Torsional angle (parameters)



Non-bonded terms





Non-bonded terms (parameters)