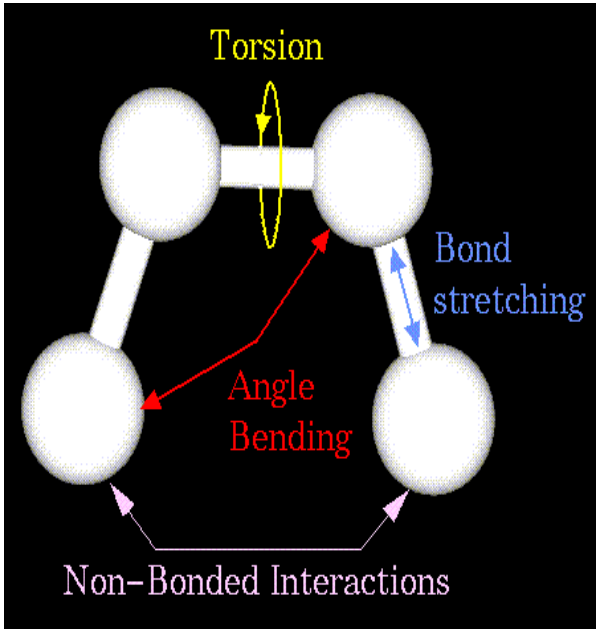
Force Field

Jeyakanthan J


Torsion
Bond
stretching
Angle
Bending
Non-Bonded Interactions

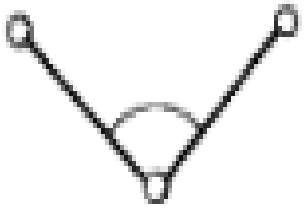
Force field

- A force field is a mathematical function which returns the energy of a system as a function of the conformation of the system.
- The forces can be written in terms of potential energy functions of various structural features such as bond lengths, bond angle, non bonded interactions etc.

Design of a Force Field

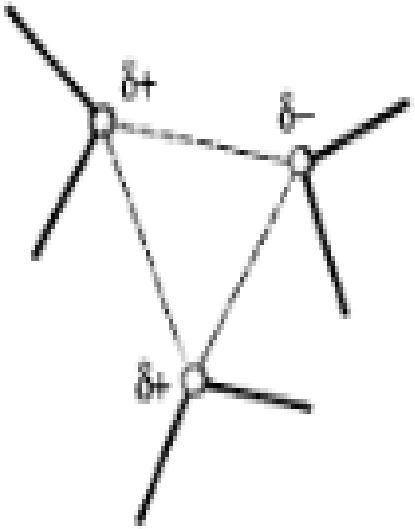
- Nuclei and electrons are lumped into atom-like particles.
- Atom-like particles are spherical and have a net charge.
- Interactions are based on springs and classical potentials.
- Interactions must be preassigned to specific sets of atoms.
- Interactions determine the spatial distribution of atom-like particles and their energies.

Bond stretching

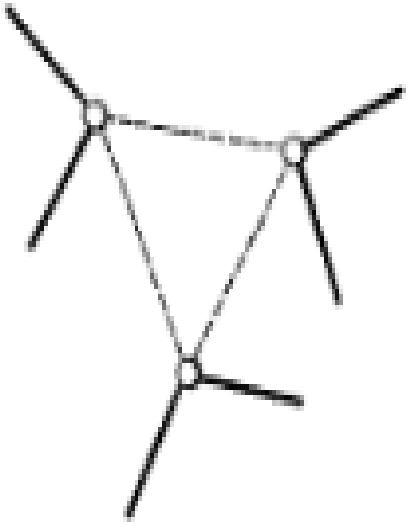


Angle bending

Bond rotation
(torsion)



Non-bonded interactions
(electrostatic)



Non-bonded interactions
(van der Waals)

Stretching & Bending

- A collection of masses connected by springs.
- By applying Hookes Law we can evaluate the energy required to stretch and bend bonds from their ideal values.

Hookes law:

Hooke's Law gives the relationship between the force applied to an unstretched spring and the amount the spring is stretched when the force is applied.

Es and Eb may be expressed as:

$$E_s = \sum_{i=1}^{N} \frac{k_i^s}{2}(l_i - l_i^0)^2$$

$$E_b = \sum_{i<j}^{M} \frac{k_{ij}^b}{2}(\theta_{ij} - \theta_{ij}^0)^2$$

- where N is the total number of bonds and M is the total number of bond angles in the molecule.
- ks and kb are the force constants for stretching and bending respectively.
- Bond stretching requires more energy than bond bending and so for a molecule being deformed most of the distortion should occur in the bond angles rather than bond lengths.

Angle Bending

- The deviation of angles from their reference values is called angle bending.
- It is described using a Hooke's law or harmonic potential:

$$\omega(\theta) = \frac{k}{2}(\theta - \theta_0)^2$$

- The contribution of each angle is characterised by a force constant and a reference value.
- Less energy is required to distort an angle away from equilibrium than to stretch or compress a bond, and the force constants are proportionately smaller.

Torsional Terms

- The bond-stretching and angle-bending terms are known as tortional terms.
- It often regarded as 'hard' degrees of free- freedom, in that quite substantial energies are required to cause significant deformations from their reference values.
- Most of the variation in structure and relative energies is due to the complex interplay between the torsional and non-bonded contributions.

- All molecular mechanics force fields use torsional potentials; it may be possible to rely upon non-bonded interactions between the atoms at the end of each torsion angle to achieve the desired energy profile.
- Torsional potentials are almost always expressed as a cosine series expansion.
- One functional form is:

$$v(\omega) = \sum_{n=0}^{N} \frac{V_n}{2} [1 + \cos(n\omega - \gamma)]$$

ω is the torsion angle.

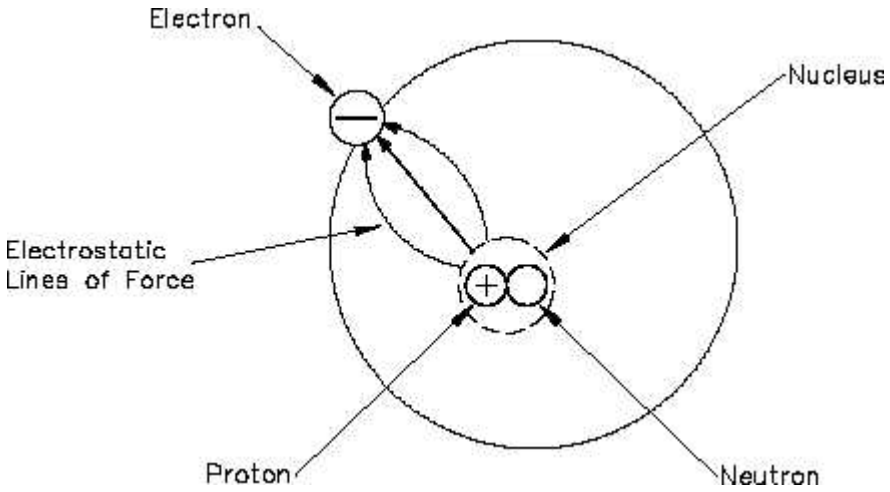
Non Bonded Interactions

- Non-bonded interactions act between atoms in the same molecule and those in other molecules.
- Force fields usually divide non-bonded interactions into two:

1. Electrostatic interactions and
2. Van der Waals interactions.

Electrostatic Interactions

- The interactions between an electron and its nucleus is known as Electrostatic Interaction.
- The force between an electrons and its nucleus is known as Electrostatic Force.
- Force that holds the electron in orbit.



The electrostatic contribution is modeled using a Coulombic potential.

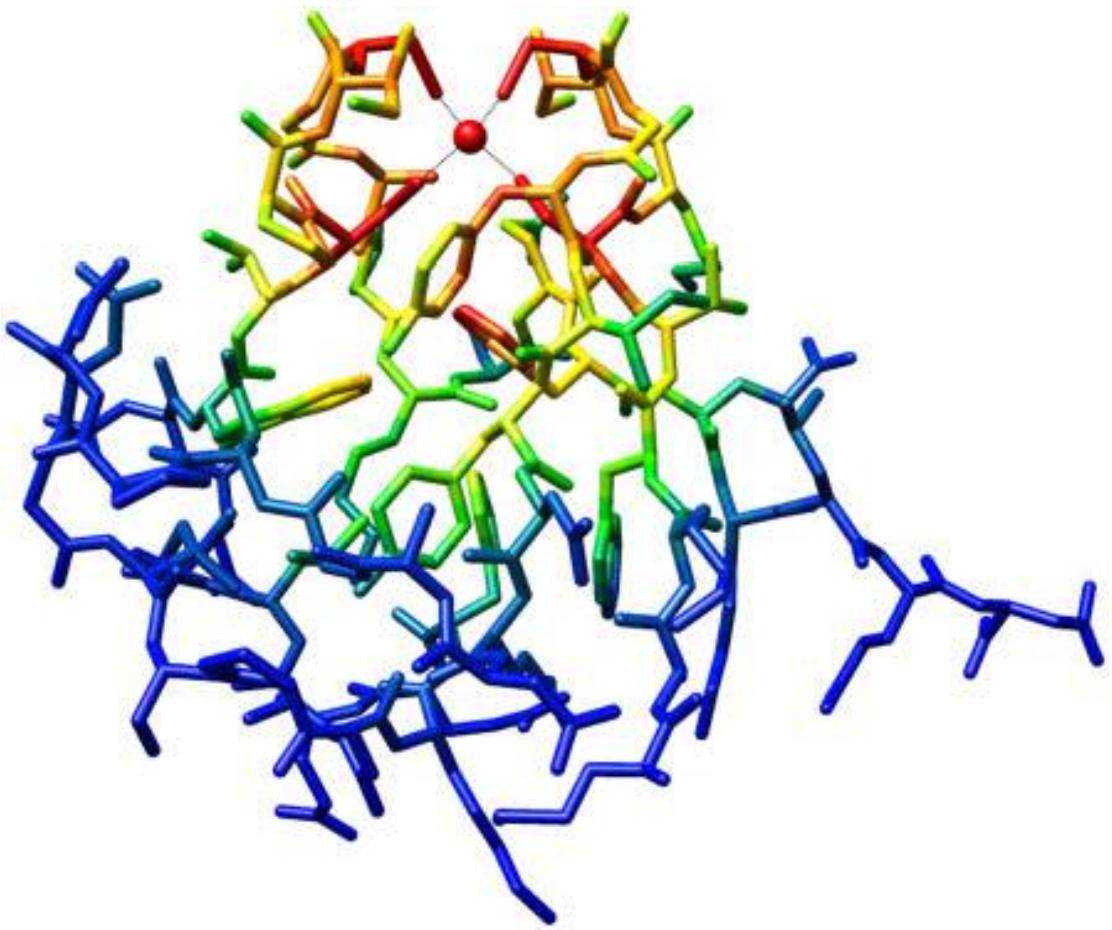
$$E_{Coul} = \sum_{i,j=1} \frac{q_i q_j}{r_{ij}}$$

Coulomb's law:

Coulomb law, is an equation describing the electrostatic force between electric charges.

The magnitude of the electrostatic force between two point electric charges is directly proportional to the product of the magnitudes of each of the charges and inversely proportional to the square of the total distance between the two charges.

Electrostatic potential interaction with metals



Differential electrostatic potential

- above 8 kT/e
- 4–8 kT/e
- 2–4 kT/e
- 1–2 kT/e
- less than kT/e

- Rubredoxin is a small electron transfer protein bearing a tetracysteine-coordinated Fe(II)-Fe(III) redox couple.
- Zn^{2+} and Ga^{3+} can each substitute into the rubredoxin active site to form structures closely isomorphous with the analogous iron charge state.
- Amide hydrogen exchange measurements were carried out on these three forms of *Pyrococcus furiosus* (*Pf*) rubredoxin, the most thermostable protein was characterized.

- Within 12 Å of the metal, the metal charge-induced change in the log ratio of the base catalyzed rate constants ($\Delta \log k_{ex}$) varies inversely with the distance between the metal and the corresponding amide nitrogen.
- The distance dependence of these data is consistent with the electrostatic potential modulating the exchange rates, by alteration of the amide nitrogen pK values.

Vanderwaal's force

- Van der Waals forces include attractions between atoms, molecules, and surfaces.
- It is the attractive or repulsive force between molecules other than those due to covalent bonds or to the electrostatic interaction of ions with one another or with neutral molecules.
- Van der Waals forces include attractions between atoms, molecules, and surfaces.
- They differ from covalent and ionic bonding in that they are caused by correlations in the fluctuating polarizations of nearby particles