

Interatomic potentials (Classical force fields)

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Atomic interactions in classical molecular dynamics

- Fundamental to making molecular simulations meaningful: evolution of molecular systems.
- Long time scales and length scales, compare with *ab-initio* calculations
- Not interested in electronic properties
- Problem does not depend critically on changes in electronic structures (no chemical reaction)
- Quick. Empirically reproduce molecular interactions: hydrophobic, H-bonds

Computational cost \sim accuracy, smaller systems

Classical FFs Semi-empirical HF DFT CI





Atomic interactions

Foundation of the studies of chemistry involve interactions between atoms that made up a molecules.

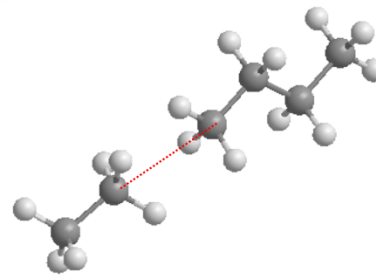
There are broadly separated into two parts:

- (1) Inter-molecular (between molecules, nonbonded)
- (2) Intra-molecular (within a molecule, bonded)

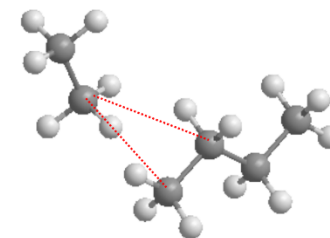


Intermolecular (non-bonded)

- DD** – Dipole-dipole interactions, including dipole-induced dipole.
- HB** – hydrogen bonding, a special case of *DD*.
- ID** – Dispersive (induced-dipole – induced-dipole), van-der-Waals type of interactions.
- HP** – hydrophobic interactions (a special case of *ID*, as between alkyl groups).
- EI** – electrostatic interactions (such as between cations and anions).
- CD** – Charge-dipole interactions (such as between ions and polar atoms).
- PS** – The π - π quadrupole interactions (such as between two aromatic rings).
- PI** – Ion- π interactions (as between a cation and an aromatic π -delocalisation system).

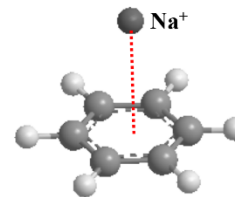


[L2]c1p:c1p



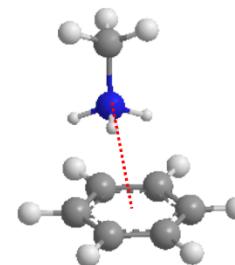
[R2]c1p:c1p-c1s:c1p

PI_6_962



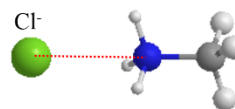
[L2]<C6>:Na962+

PI_6_47



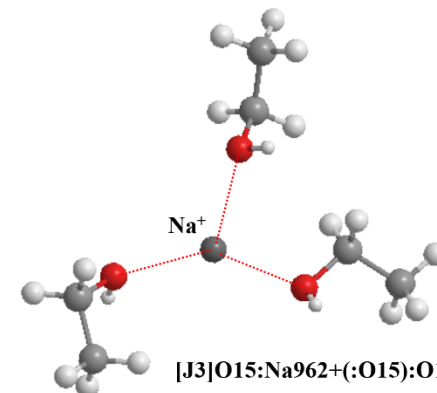
[L2]<C6>:N47+

EI_47_963



[L2]N47+:Cl963-

CD_15_963

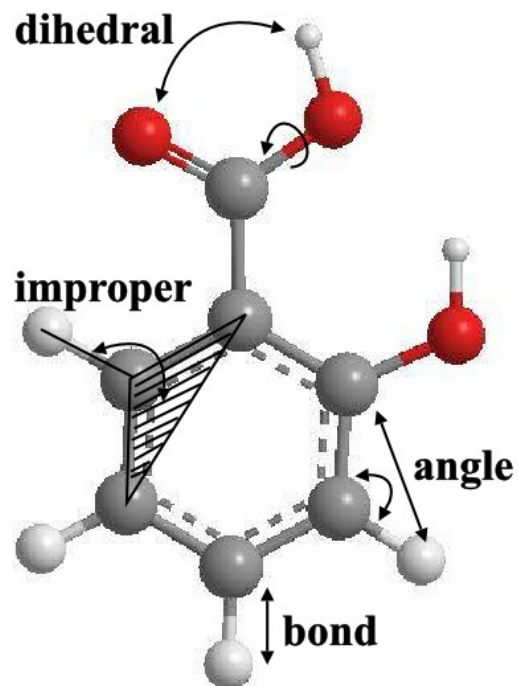


[J3]O15:Na962+:(O15):O15

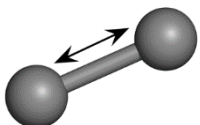
Intra-molecular (bonded interactions)

Short-range, within the molecule and maintaining the geometrical structure of the molecule.

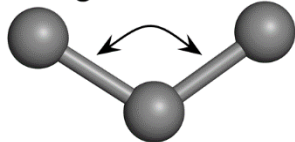
Salicylic acid



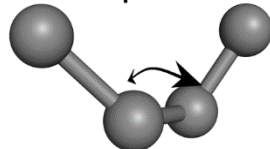
Bond vibration



Angle vibration



Torsion potentials



Basic components:

- Bond (two-body)
- Angle (three-body)
- Dihedral (four-body)
- Improper (four body)
- Urey-Brdley (1-3 two body)

Can also have cross-components:

- Bond-bond,
- Bond-angle,
- Angle-angle, etc.

Force fields

The atomic interactions (both inter- and intra-), also known as the potentials, collectively form a **force field (FF)**.

Potentials often contain (usually implicitly) a number of physical approximations – they are related to *models* of system behaviour. They can be *generic* to a class or *specific* for a material.

A force field (FF) is modelled classically as some mathematical descriptions of forces and energies between atoms, in terms of atomic positions

$$FF = pot1(x,y,z) + pot2(x,y,z) + \dots + potn(x,y,z)$$

Where $pot(x,y,z)$ is a mathematical function of an interaction component. Each Function also contains some constants (potential parameters) that are **adjusted** such that the potential function **approximately** represent the chemical behaviour of the interaction component.

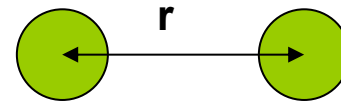
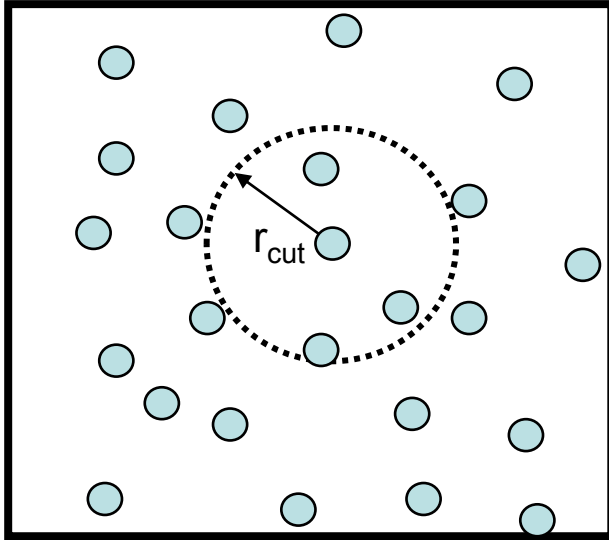
Molecular modelling

Consider a noble gas such as argon. The only interaction component is induced dipole dispersive (van-der-Waals) interaction.

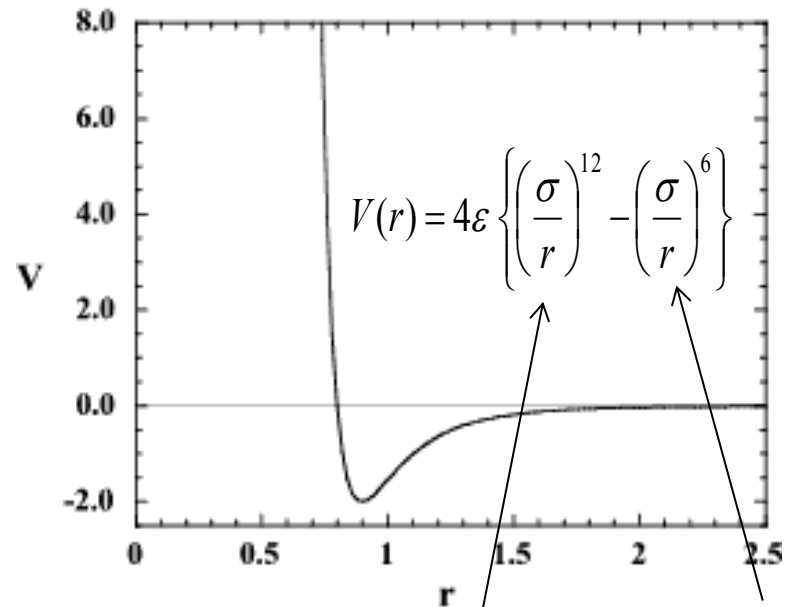
Atoms represented as spheres



Sphere - sphere interactions represented by some mathematical functional forms.



Van-der-Waals interactions.



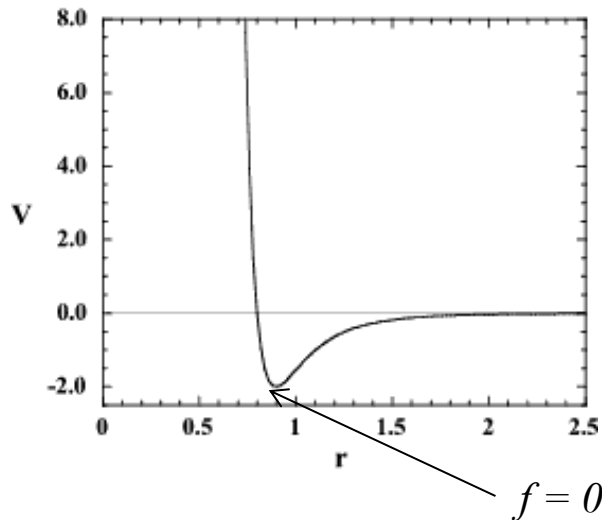
Overlap of electron cloud

Interactions due to induced dipoles

$$V = Fr$$

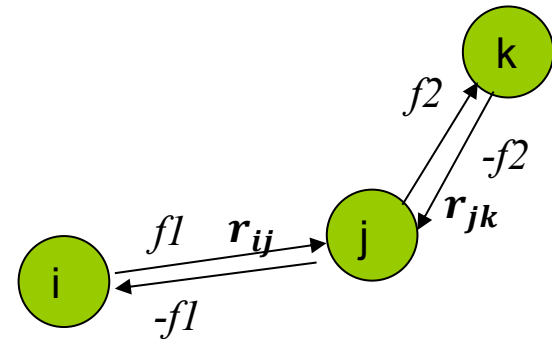
$$F = \frac{V}{r}$$

$$\Delta F = -\frac{dV}{dr}$$



$$V(r) = 4\epsilon \left\{ \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right\}$$

$$\begin{aligned}
 f &= \frac{dV}{dr} \\
 &= \frac{24\epsilon}{r} \left\{ 2 \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right\}
 \end{aligned}$$



- The slope of the graph at a given r indicates the magnitude and direction of the force exerts on a sphere ('chemical forces').
- The total force exerts on a sphere (i) is the contribution of individual forces from other neighbouring spheres that exert on that sphere (i).

Once you know the resultant forces for every atom, you can determine how the atoms move.

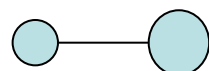
Organic molecules

$$E_{(total)} = E_{(bonded)} + E_{(cross-terms)} + E_{(nonbonded)}$$

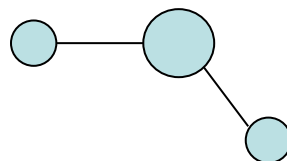
$$E_{(nonbonded)} = E_{(vdw)} + E_{(coulomb)} + E_{(H-bond)}$$

$$E_{(bonded)} = E_{(bond)} + E_{(angle)} + E_{(torsion)} + E_{(oop)} + E_{(ub)}$$

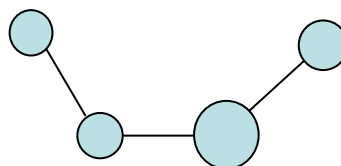
For a 'typical' organic FF (molecular mechanics (MM)):



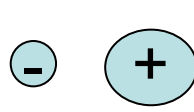
$$V(b) = k_b(b - b_0)^2 \quad (\text{bond, harmonic spring})$$



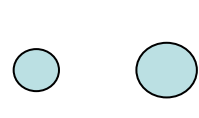
$$V(\theta) = k_a(\theta - \theta_0)^2 \quad (\text{angle, harmonic spring})$$



$$V(\varphi) = \sum_n k_n [1 + \cos(n\varphi - \delta)] \quad (\text{torsion, fourier series})$$



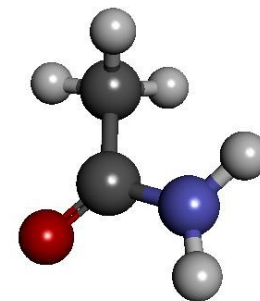
$$V(r_{ij}) = \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{|r_{ij}|} \quad (\text{Coulombic})$$



$$V(r_{ij}) = \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^6}$$

(vdw, Lennard-Jone 12-6)

Special DD interactions.
Split from vdw.



Parameters fitted on
individual potential functions
to model the behaviour and
structure of a molecule

Parameter fittings

- What are you going to fit to?
 - Experiment:
 - How good is the data you are fitting to?
 - Is bulk crystal data good enough to describe your situation?
 - What data are you using to validate the results?
 - Calculation:
 - Were the calculations done properly?
 - Does the method used include the effects you are fitting to?
 - How comprehensive is the set of configurations you have?
 - Does the simulation data you have enable you to fit to the relevant length and timescales?
- What functional form are you going to use?

(Need some elements of intuition. As long it works, who care?)

Force field qualities

Specific (*many parameters, limited applicability (specific class of molecules, high accuracy)*)

Generic (*fewer parameters, more generalizations, wide applicability, poor accuracy*)

Easiest to use in point-and click commercial software (Materials Studio, Chem3D, MacroModel, etc)

Often fit to a range of test molecules.

Many force fields employ similar mathematical equations but differ in the parameters used in the equations.

Care when mixing parameters between force fields.

CHARMM fitting scheme

Pure solvents:
heats of vapourisation,
Molecular volumes,
Heat capacities

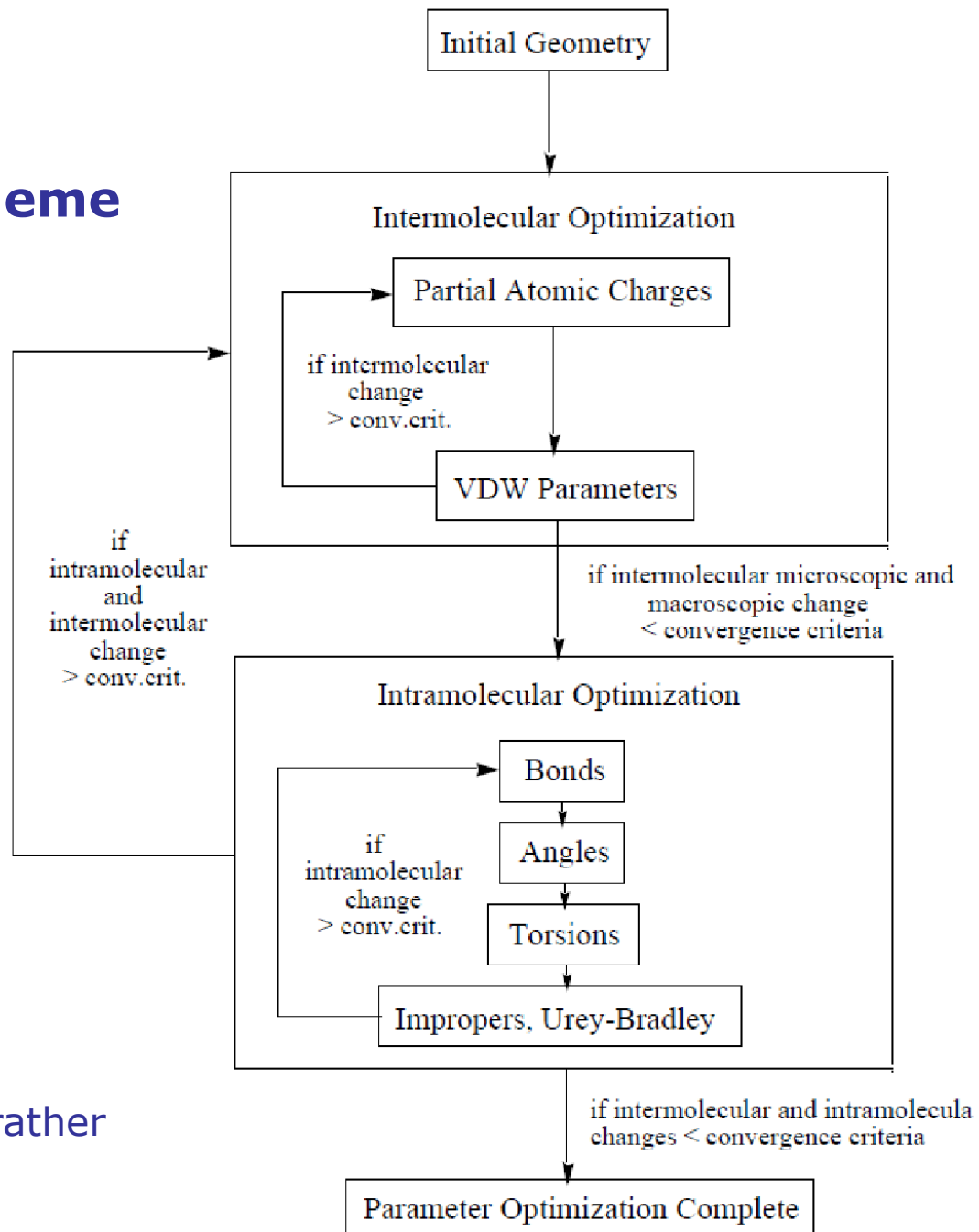
Aqueous:
Free energy of solvation
Partial molar volumes

Crystals
Heats of sublimation
Lattice parameters

Force constants:
IR, Raman, *ab initio*

Torsional surfaces:
Microwave, NMR,
Ab initio

Parameter fittings more of an art rather than science! Labour-intensive.



Partial charges and atom types

Molecular electronic density can be achieved by high-level QM calculations, but to translate into MD description is not easy – partial charges. Not an experimental observables

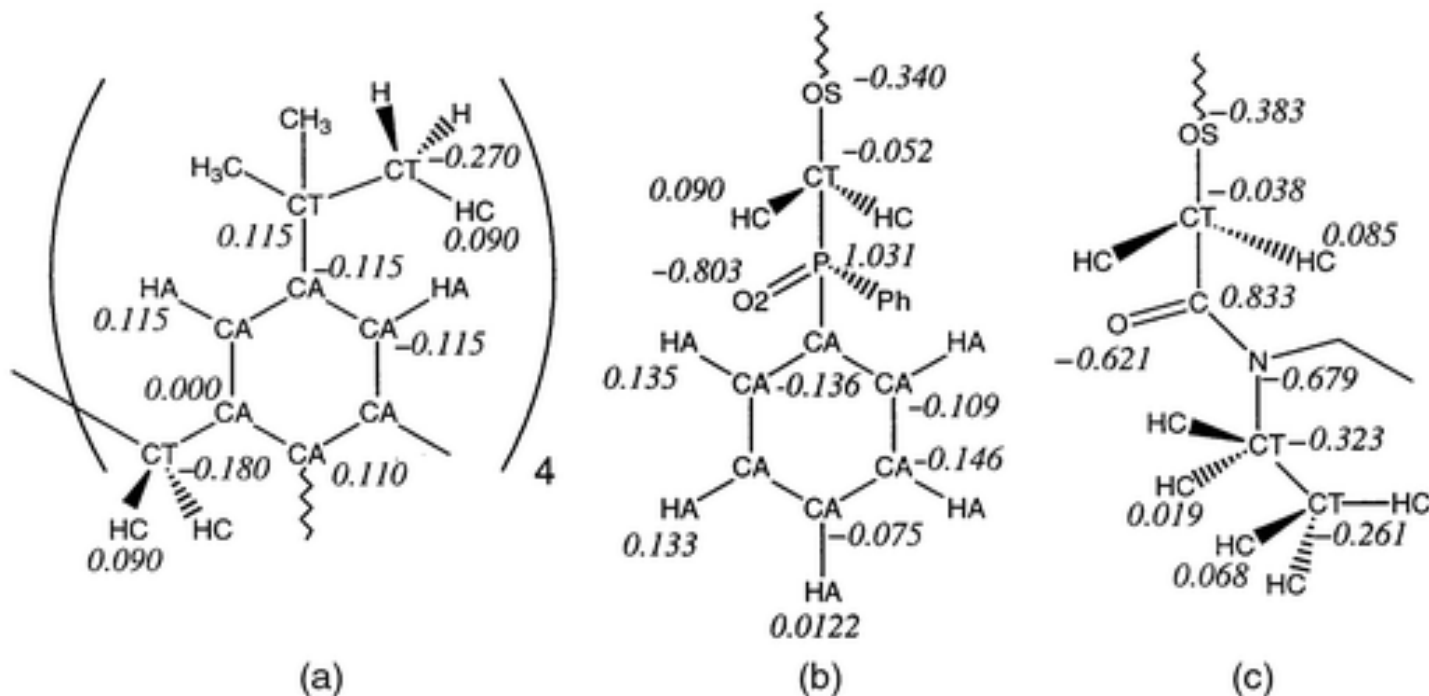
Difference in electronegativity between atoms – unequal charge distribution.

Different chemical behaviour for same element.

Assign different symbols (**atom types**) to a same element.

Procedure to do this is called **atom typing**....HOW DO YOU DO THIS?

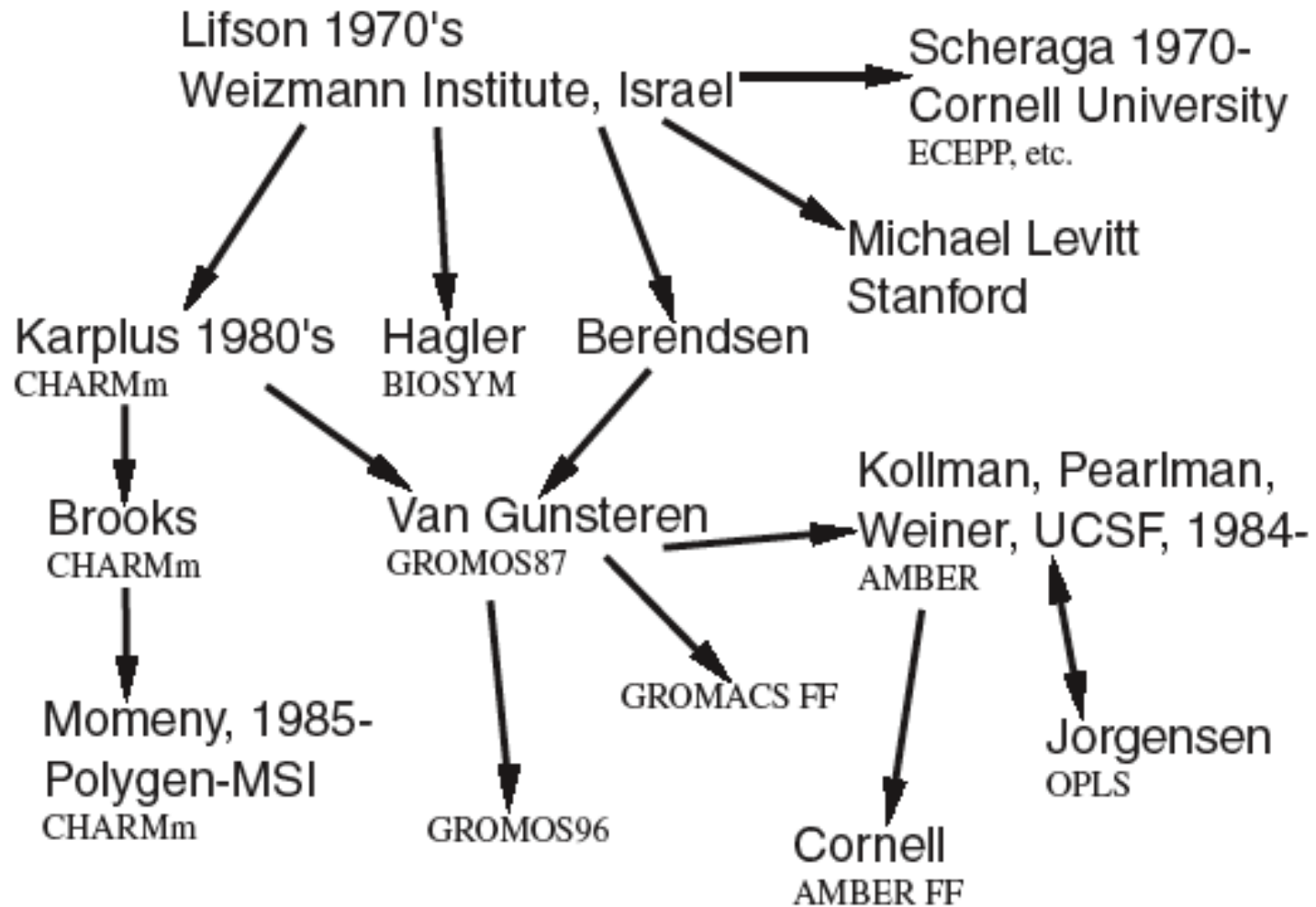
$$V(r_{ij}) = \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{|r_{ij}|}$$



Since there is no such thing as a fractional electron, therefore there is no perfect method to derive the partial atomic charges



FF family tree



Some popular FF for biomolecules and organic molecules simulations

- CHARMM (Chemistry at HARvard using Molecular Mechanics)
- AMBER (Assisted Model Building with Energy Refinement)
- OPLS (Optimized Parameters for Large-scale Simulations)
- MMFF (the Merck Molecular Force Field)
- MM2, MM3, MM4 – Allinger *et. al.*
- PCFF, CVFF
- UFF (Universal Force Field)
- DREIDING
- Commercials (OPLS3, COMPASS)

Lots of variations: CHARMM22, CHARMM36, Amber Glycam, CHARMM CGenFF, OPLS-AA/L, OPLS-AA/M, OPLS-CL_P, etc

Force field class

Class 1: CHARMM, AMBER, OPLS – fits well to thermodynamic Properties in condensed phase.

Use only a few potential forms. Even then, still quite a number of parameters

Intramolecular

$$\begin{aligned} & \sum_{\text{bonds}} K_b (b - b_o)^2 + \sum_{\text{angles}} K_\theta (\theta - \theta_o)^2 + \sum_{\text{torsions}} K\phi (1 + \cos(n\phi - \delta)) \\ & + \sum_{\text{impropers}} K_\varphi (\varphi - \varphi_o)^2 + \sum_{\text{Urey-Bradley}} K_{UB} (r_{1,3} - r_{1,3,o})^2 \end{aligned}$$

Intermolecular

$$\sum_{\text{electrostatics}} \frac{q_i q_j}{r_{ij}} + \sum_{\text{VDW}} \epsilon_{ij} \left[\left(\frac{R_{\text{min},ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{\text{min},ij}}{r_{ij}} \right)^6 \right]$$



Class 2: CVFF, PCFF, MM3, MM4

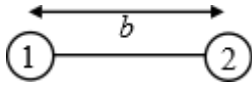
$$\begin{aligned}
 & \sum_{\text{bonds}} \left[K_{b,2} (b - b_o)^2 + K_{b,3} (b - b_o)^3 + K_{b,4} (b - b_o)^4 \right] \\
 & + \sum_{\text{angles}} \left[K_{\theta,2} (\theta - \theta_o)^2 + K_{\theta,3} (\theta - \theta_o)^3 + K_{\theta,4} (\theta - \theta_o)^4 \right] \\
 & + \sum_{\text{dihedrals}} \left[K_{\phi,1} (1 - \cos \phi) + K_{\phi,2} (1 - \cos 2\phi) + K_{\phi,3} (1 - \cos 3\phi) \right] \\
 & + \sum_{\text{impropers}} K_{\chi} \chi^2 \\
 & + \sum_{\text{bonds}} \sum_{\text{bonds}'} K_{bb'} (b - b_o)(b' - b_o') + \sum_{\text{angles}} \sum_{\text{angles}'} K_{\theta\theta'} (\theta - \theta_o)(\theta' - \theta_o') \\
 & + \sum_{\text{bonds}} \sum_{\text{angles}} K_{b\theta} (b - b_o)(\theta - \theta_o) \\
 & + \sum_{\text{bonds}} \sum_{\text{dihedrals}} (b - b_o) \left[K_{\phi,b1} \cos \phi + K_{\phi,b2} \cos 2\phi + K_{\phi,b3} \cos 3\phi \right] \\
 & + \sum_{\text{bonds}'} \sum_{\text{dihedrals}} (b' - b_o') \left[K_{\phi,b'1} \cos \phi + K_{\phi,b'2} \cos 2\phi + K_{\phi,b'3} \cos 3\phi \right] \\
 & + \sum_{\text{angles}} \sum_{\text{dihedrals}} (\theta - \theta_o) \left[K_{\phi,\theta1} \cos \phi + K_{\phi,\theta2} \cos 2\phi + K_{\phi,\theta3} \cos 3\phi \right]
 \end{aligned}$$

Slower. More realistic.
Reproduce various
vibrational frequencies.

Emphasis on reproduction
of geometries and dipole
moments.

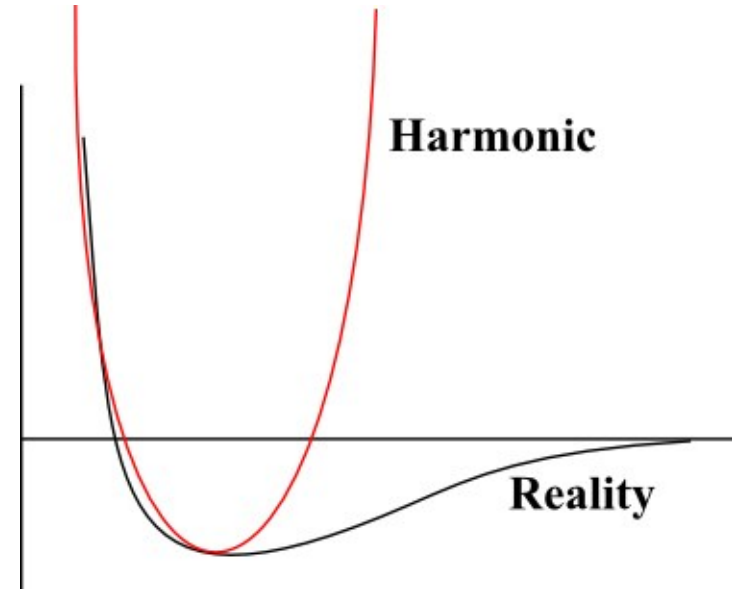
Does not mean better.
Not much difference in
terms of molecular structures
compare with class I.

Bond potential



$$V(b) = k_b(b - b_0)^2 \quad \text{harmonic}$$

$$V(b) = D_e[1 - e^{-\alpha(b-b_0)}]^2 \quad \text{Morse}$$



Harmonic: approximation.

It is unbreakable. They are suitable only for distances close to equilibrium point close to room temperature.

This is the reason, in classical , simulations, no chemical reaction is permitted.

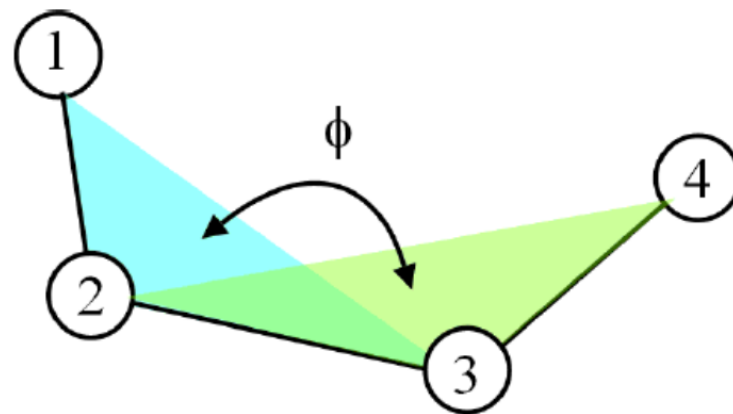
Morse is a better approximation, which is anharmonic (need three parameters).

(same for angle potential)

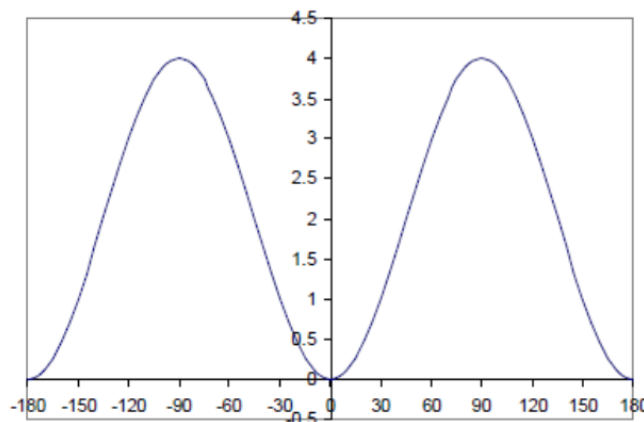


Torsion (dihedral) term

- Rotation about chemical bonds. Torsional potentials model the effect of steric hindrance in macromolecules on the molecular shape.

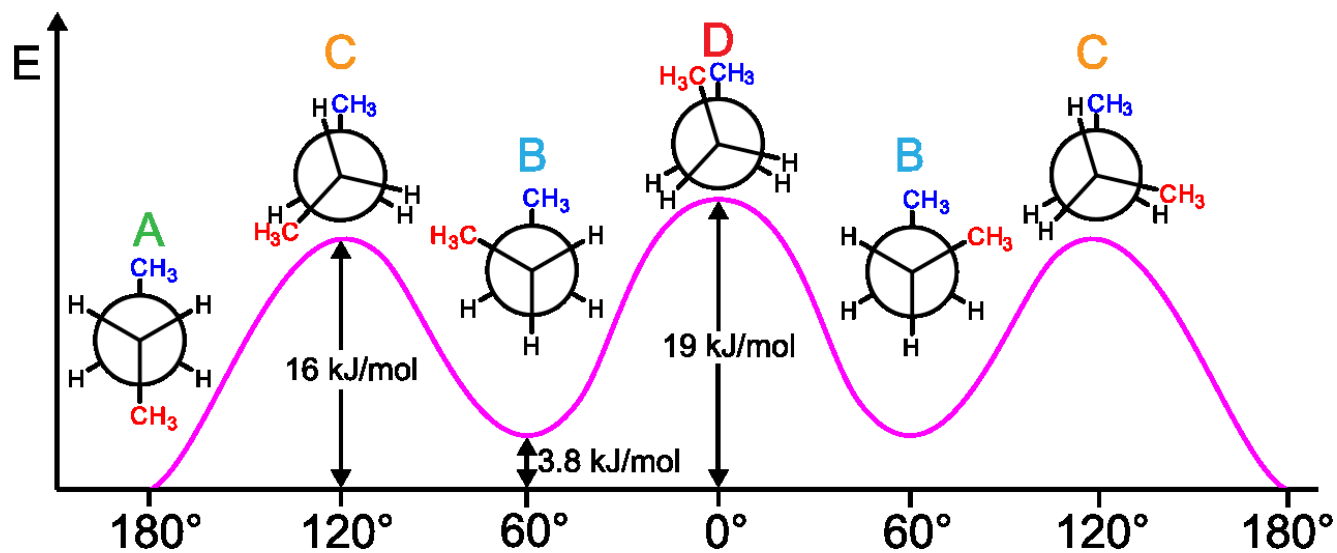
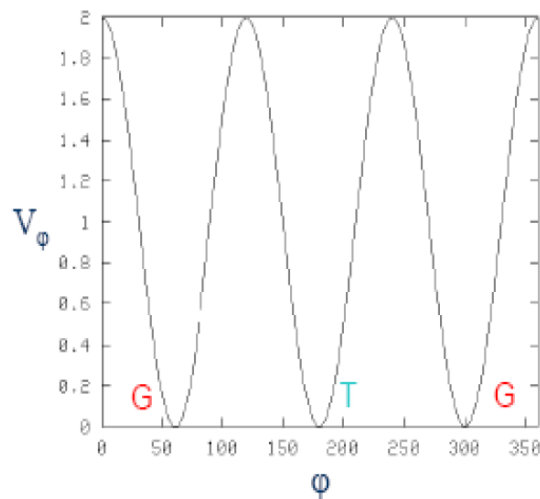


$$\varphi(\phi) = \sum_{n=0}^N \frac{V_n}{2} [1 + \cos(n\phi - \gamma)]$$



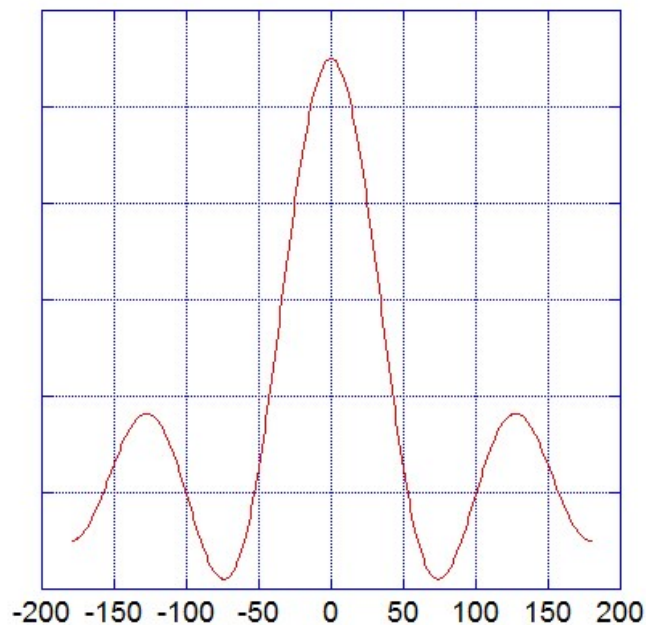
$$V_n = 4, n = 2, \gamma = 180$$

Using $n = 3$ to model *trans* and *gauche* states



...but in reality, the energies between gauche and trans can be different. To model this, the torsion function can be expanded with additional terms, each with its unique contribution to the rotational energy:

$$V(\varphi) = \frac{k_1}{2}(1 + \cos\varphi) + \frac{k_2}{2}(1 + \cos 2\varphi) + \frac{k_3}{2}(1 + \cos 3\varphi)$$

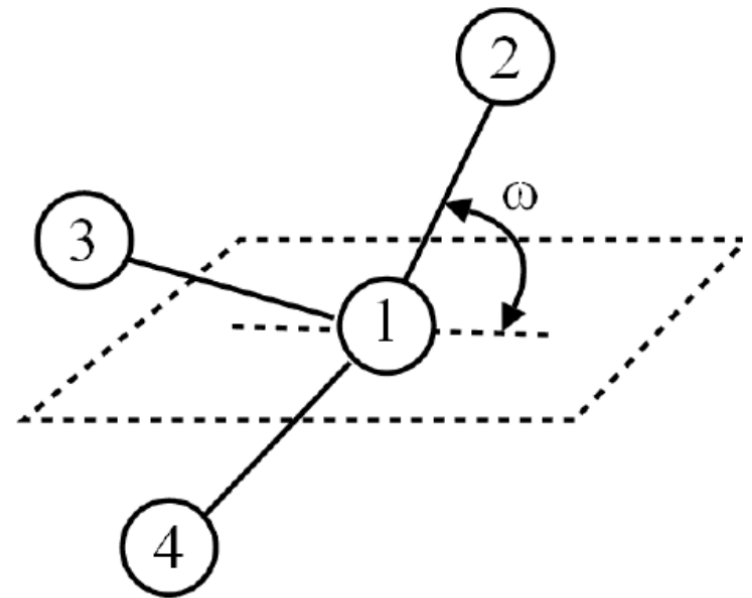




Improper term

intended to maintain a particular **geometry** in the system.

- *Improper* because the sequence of the atoms to define the angle is not that for a proper torsion. The angle is between the plane defined by 1-3-4 and the bond 1-2



$$\varphi(\omega) = k(1 - \cos(\omega))$$

For example, to keep planar geometry due to sp² hybridisation (C=O carbonyls)

Non-bonded (non-electrostatic) term

- Assume that interaction is between pairs of atoms and that it depends only on the interatomic distance. Also used for simple ionic materials

- Many different types of functional form. The commonest are

- Lennard-Jones*

$$V_{\text{non-bond}} = \varepsilon \left(\left[\frac{\sigma}{r} \right]^{12} - \left[\frac{\sigma}{r} \right]^6 \right)$$

Electron repulsion due
To Pauli exclusion principle.

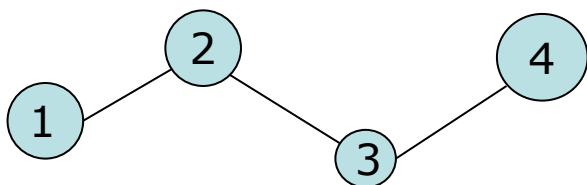
- Buckingham*

$$V_{\text{nonbond}} = A \exp(-r / \rho) - Cr^{-6}$$

Dispersive
Instantaneous dipole
due to electron cloud
fluctuation.

- Coulombic** terms also of this type but special methods needed to sum them up.

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In covalent, organic molecules,
1-2, 1-3 interactions are ignored.
A constant scaling factor is needed for 1-4

Non-bonded mixing rules

- In complex (particularly bio) systems, there are a large number of interactions, often too many to fit them all.
- Missing non-bonding interactions usually estimated using *mixing rules*. These have minimal justification but often work well enough. Can fail when the fitting of different parts of the potential corresponds to different types of bonding (e.g. a biomolecule on a ceramic surface)

- *Lennard-Jones* $\epsilon_{AB} = \sqrt{\epsilon_{AA}\epsilon_{BB}}$ $\sigma_{AB} = \frac{1}{2}(\sigma_{AA} + \sigma_{BB})$
(arithmetic)

- *Buckingham* $A_{AB} = \sqrt{A_{AA}A_{BB}}$ $C_{AB} = \sqrt{C_{AA}C_{BB}}$
(geometric)



$$\frac{1}{\rho_{AB}} = 2 \frac{(\rho_{AA} + \rho_{BB})}{\rho_{AA}\rho_{BB}}$$

Non-bonded cut-offs

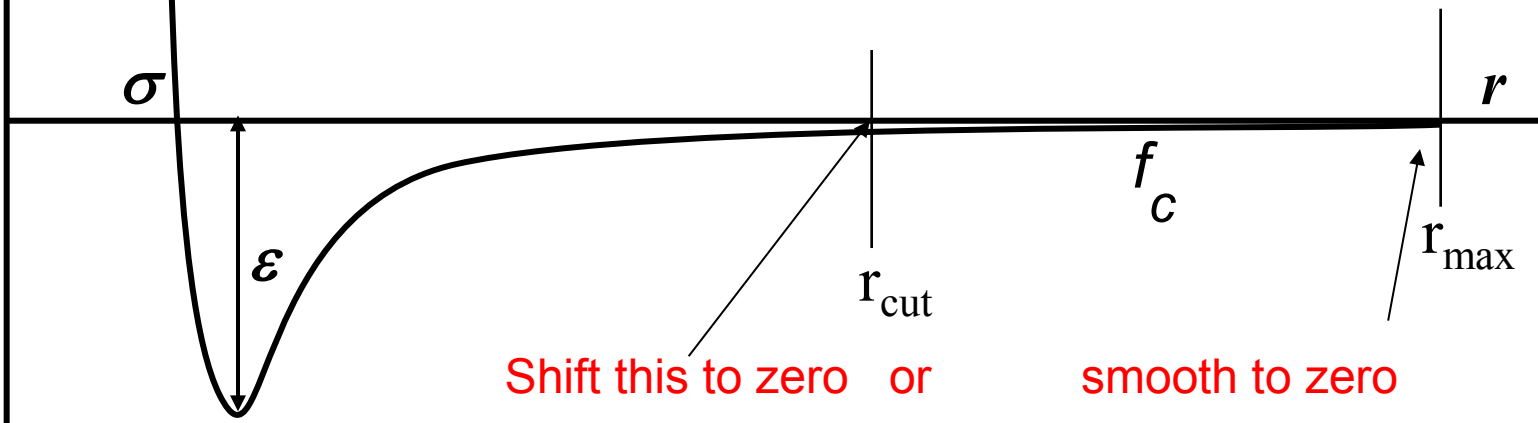
- Few potentials decay to zero at a convenient length-scale. How they are ignored beyond a given distance (and what that distance is) is important since it is part of the definition of the potential function.
- Simplest to ignore the potential beyond a set distance. Can give strange behaviour in the dynamics if forces at the “step” are large enough to contribute significantly.
- Use a smoothing function to take the potential to zero over a short distance. Many examples; a simple one is

$$\begin{aligned} f_C(r) &= 1 & r < R - D \\ f_C(r) &= \frac{1}{2} - \frac{1}{2} \sin \left\{ \frac{\pi}{2} (r - R) / D \right\} & R - D < r < R + D \\ f_C(r) &= 0 & r > R + D \end{aligned}$$

$V(r)$

$$V(r_{ij}) = 4\varepsilon \left\{ \left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right\} f_c$$

Note that the using a potential cut-off, r_{cut} , implies a discontinuity in f which can be avoided by using a shifted potential or a smoothing function.



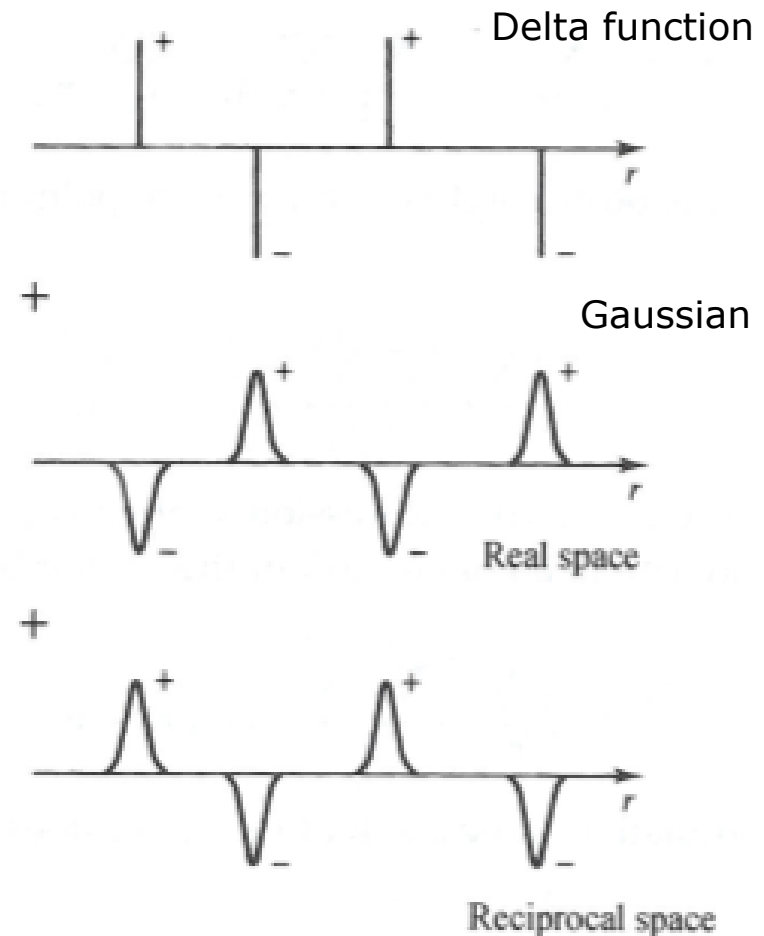
Electrostatic interaction

$$V(r_{ij}) = \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{|r_{ij}|}$$

Decays as $\sim 1/r$. Slow convergence. Cannot use traditional cut off in periodic systems. Have to include all charges in periodic images.

Use of Ewald summation: summation of energy equivalent summation in Fourier space.

The method offers an elegant solution to solving the full electrostatic problem by splitting it in two parts – one in *real space* and one in *reciprocal space*. In real space, complying with the cutoff concept, a convenient screening function is added around all charges to make their interactions decay very fast at r_{cut} . The added screening functions can be subtracted in reciprocal space due to the periodic boundary condition by using *Fourier transforms*.



Non-classical potentials

Note that general biological FFs do not allow breaking of bonds

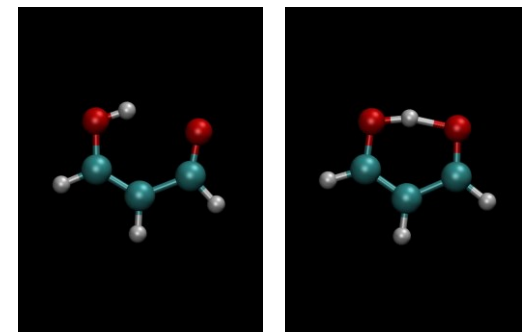
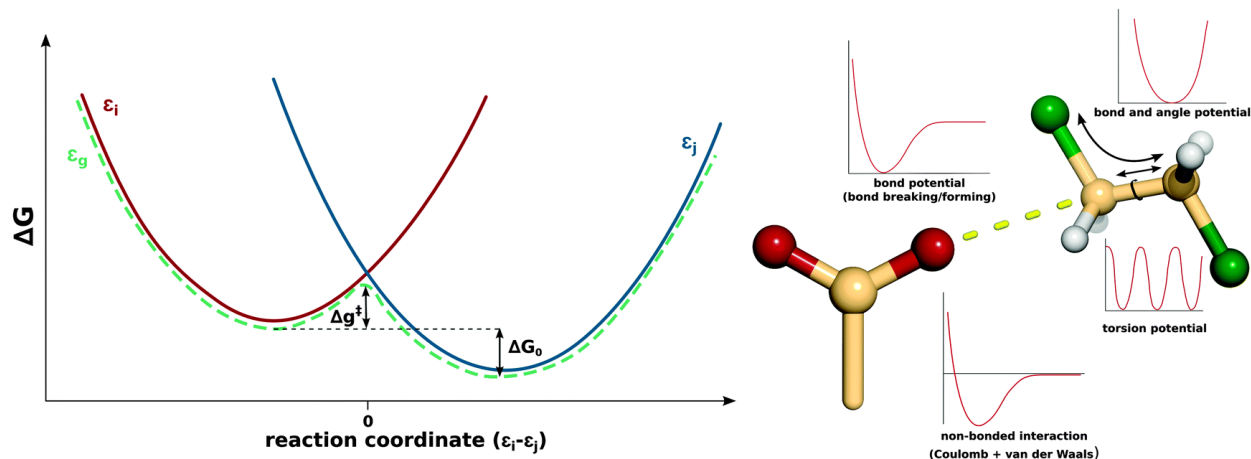
- Models such as the **reactive forcefield** use ideas of *bond order* to build a model of the interaction.
- Bond orders (e.g. sigma, pi etc) are obtained from empirical expressions parametrised to fit quantum calculations of bond strengths and distances. These may need to be adjusted to ensure chemical sense.

$$BO_{ij} = \sum_{\alpha} \exp \left(A_{\alpha} \left(\frac{r_{ij}}{r_{ij}^0} \right)^{n_{\alpha}} \right)$$

- These give a measure of the strength or weakness of a bond and are used to scale the angle-bending and torsion terms.

Empirical Valence Bond

Reactive dynamics for bond breaking and (re)making via product and reactant mixing terms



malonaldehyde

Reactive surface is defined as the lowest adiabatic surface, by diagonalization of the non-reactive, diabatic Hamiltonian matrix, for state 1 and state 2.

$$\mathbf{H} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

H_{11} H_{22} Energies of classical force fields

$H_{12} = H_{21}$ Coupling elements, reproduce experimental results, or by DFT.

Polarization effect

$$\mu = \alpha E$$

Distribution of electron depends on the environment, even more so in condensed phase, due to local electric field effect, which will induce a dipole moment. Fixed partial charges cannot fully account for this.

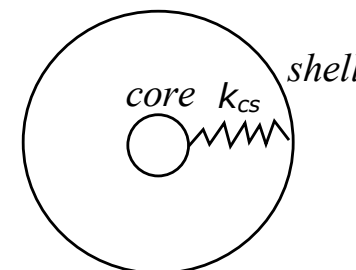
Important contribution to energetic and directionality of H-bond

Interactions of ions in non-polar solvents and aromatic systems.

Charge redistribution can be remodelled by taking polarization effect into account.

Physical phenomena is there but how important it is in biology?

What is the correct scientific approach?



1. Drude mode (core-shell) – separate charge into core and shell connected by a harmonic spring with force constant related to the atomic polarizability.

$$\alpha = q^2/k$$

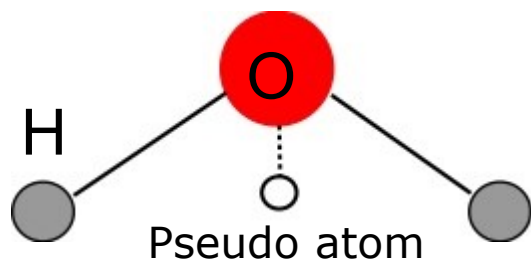
2. Fluctuating charge equilibration – base on electronegativity equalization principle. Charges allow to fluctuate until instantaneous electronegativity are equal.

Non-Centered Point Charge Approximation

By add off-nucleus point charges can improve fit to QM.

Point charge (pseudo atoms) to represent lone pairs

Model π -stacking and cation- π interactions.



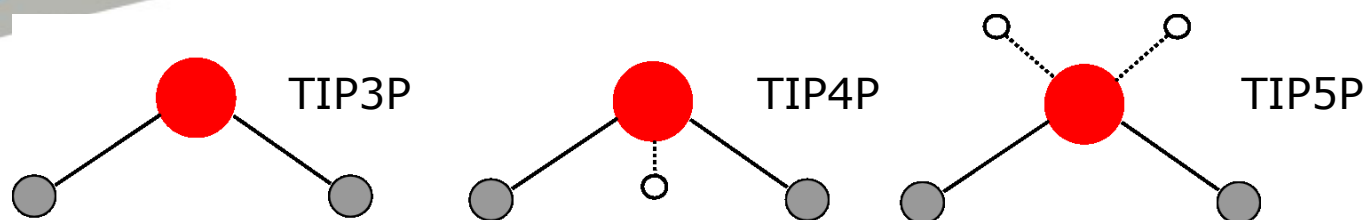
TIP4P water model.

Point charge is at the pseudo atom, but the vdw sphere is still centered at oxygen.

The pseudo atom position is fixed relative to the atoms.



Water models



Model	Dipole Moment	Dielectric Constant	Self-diffusion	Config. Energy	Density Max (C)	Expansion Coefft
Expt	2.95	78.4	2.30	-41.5	+3.98	2.53
SPC	2.27	65	3.85	-41.0	-45	7.3
TIP3P	2.35	82	5.19	-41.1	-91	9.2
TIP4P	2.18	53	3.29	-41.8	-25	4.4
TIP5P	2.29	81.5	2.62	-41.3	+4	6.3
POL5/TZ	2.712	98	1.81	-41.5	+25	-

www.lsbu.ac.uk/water/models.html

Coarse grain models

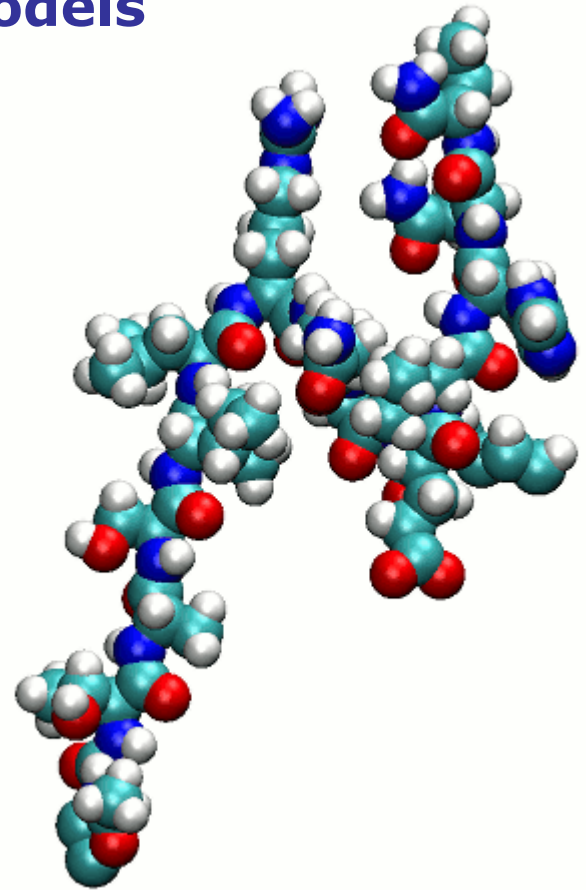
Several atoms fused into a single site interactions.

The simplest one is the fusion of hydrocarbon groups (united atom models). Polar atoms remain the same.

Fastest degrees of freedom are naturally removed, and reduce the number of atoms in calculations.

Timesteps can increase > 5 fs.

However some atomic details are lost.



FAQ in FFs

What's the best force field? What do you mean best?

Which FF schemes to use?

How and when can I use a certain set of parameters?
- issue of transferability.

How do you know what parameters to assign to which atoms?

You should also ask this:

- is my model correct? Is charge state correct (especially for proteins)?
- Is it feasible to run in MD?

Force field model setup

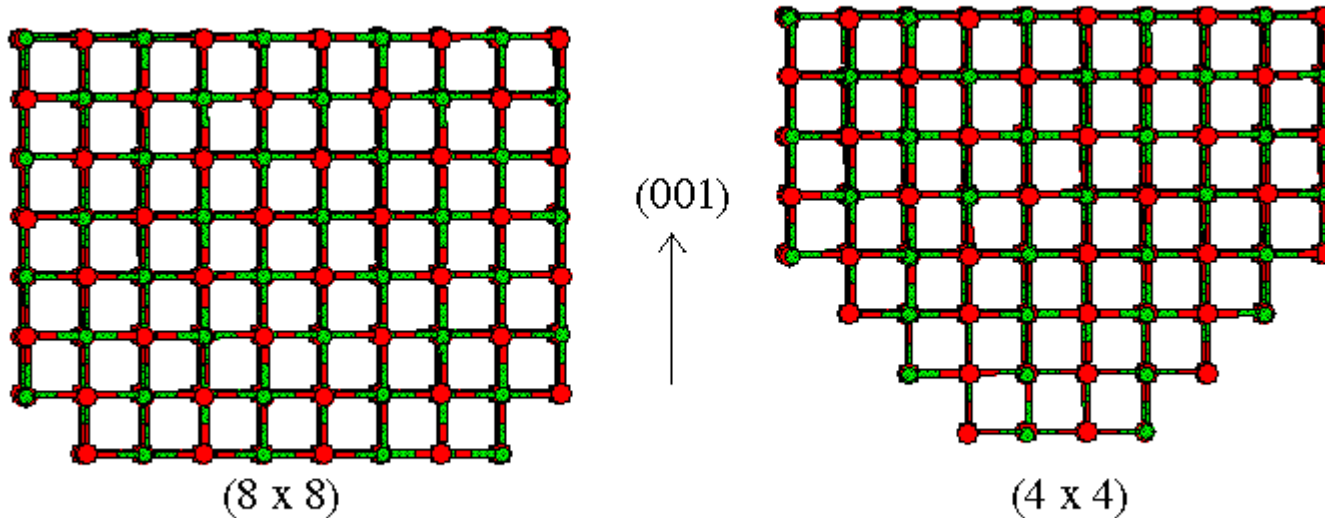
$$E(\text{total}) = E(\text{valence}) + E(\text{cross-terms}) + E(\text{nonbonded})$$

$$E(\text{nonbonded}) = E(\text{vdw}) + E(\text{coulomb}) + E(\text{H-bond})$$

$$E(\text{valence}) = E(\text{bond}) + E(\text{angle}) + E(\text{torsion}) + E(\text{oop}) + E(\text{ub})$$

E is expressed by some kind of equations and parameters can be ambiguous.

Force fields for MgO, NaCl, simple ionic crystals - easy



$$E(\text{total}) = E(\text{vdw}) + E(\text{coulomb})$$

$$E(\text{valence}) = 0$$

Three descriptions: Mg^{2+} with Mg^{2+} , Mg^{2+} with O^{2-} and O^{2-} with O^{2-}

Mg

+2

O

-2

MgO – rigid ion model

atoms 24

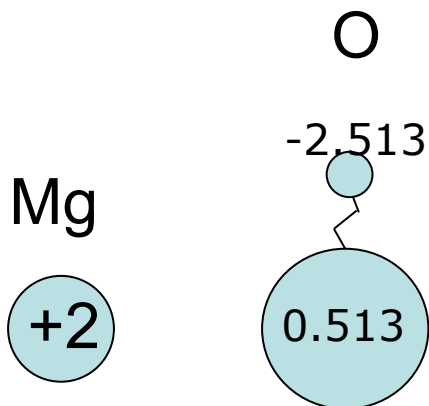
Mg3	24.30500	2.00000	12	0
O10	15.99940	-2.00000	12	0

finish

vdw 3

Mg3	Mg3	buck	0.0000	0.0000	0.0000
O10	Mg3	buck	26566.2720	0.3065	0.0000
O10	O10	buck	524868.3600	0.1490	667.8466

close



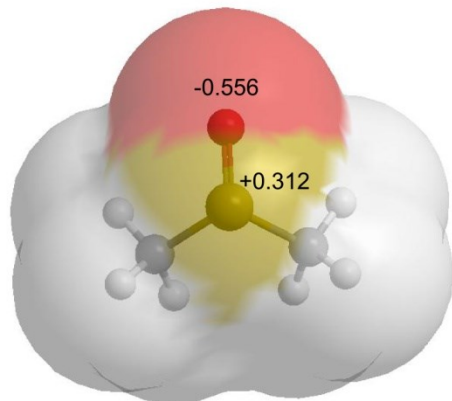
```
atoms 24
Mg1c 24.30500 1.58000 6 0
Mg1s 0.00000 0.42000 6 0
O2c 15.99940 0.51300 6 0
O2s 0.00000 -2.51300 6 0
shell 12
  1 7 8070.19695
  2 8 8070.19695
  3 9 8070.19695
  4 10 8070.19695
  5 11 8070.19695
  6 12 8070.19695
 13 24 473.44233
 14 19 473.44233
 15 20 473.44233
 16 21 473.44233
 17 22 473.44233
 18 23 473.44233
finish
vdw 10
Mg1c Mg1c buck 0.0000 0.0000 0.0000
Mg1s Mg1c buck 0.0000 0.0000 0.0000
O2c Mg1c buck 0.0000 0.0000 0.0000
O2s Mg1c buck 0.0000 0.0000 0.0000
Mg1s Mg1s buck 0.0000 0.0000 0.0000
O2c Mg1s buck 0.0000 0.0000 0.0000
O2s Mg1s buck 56666.4808 0.2610 0.0000
O2c O2c buck 0.0000 0.0000 0.0000
O2s O2c buck 0.0000 0.0000 0.0000
O2s O2s buck 585.9800 0.6937 745.3315
close
```

Can remove in
DL_POLY



Simple covalent molecules - bearable

For example: dimethyl sulphoxide



$$E(\text{total}) = E(\text{valence}) + E(\text{cross-terms}) + E(\text{nonbonded})$$

$$E(\text{valence}) = E(\text{bond}) + E(\text{angle}) + E(\text{torsion}) + E(\text{oop}) + E(\text{ub})$$

$$U(b) = k(b - b_0)^2$$

atoms 10

HD	1.00797	0.09000	1
HD	1.00797	0.09000	1
HD	1.00797	0.09000	1
CD	12.01115	-0.14800	1
HD	1.00797	0.09000	1
HD	1.00797	0.09000	1
HD	1.00797	0.09000	1
CD	12.01115	-0.14800	1
SD	32.06400	0.31200	1
OD	15.99940	-0.55600	1

bonds 21

harm	4	1	644	1.11000
harm	4	2	644	1.11000
harm	4	3	644	1.11000
harm	8	5	644	1.11000
harm	8	6	644	1.11000
harm	8	7	644	1.11000
harm	4	9	480	1.80000
harm	8	9	480	1.80000
harm	9	10	1080	1.53000
-126	1	8	96195	129.03
-126	1	10	33433	84.716

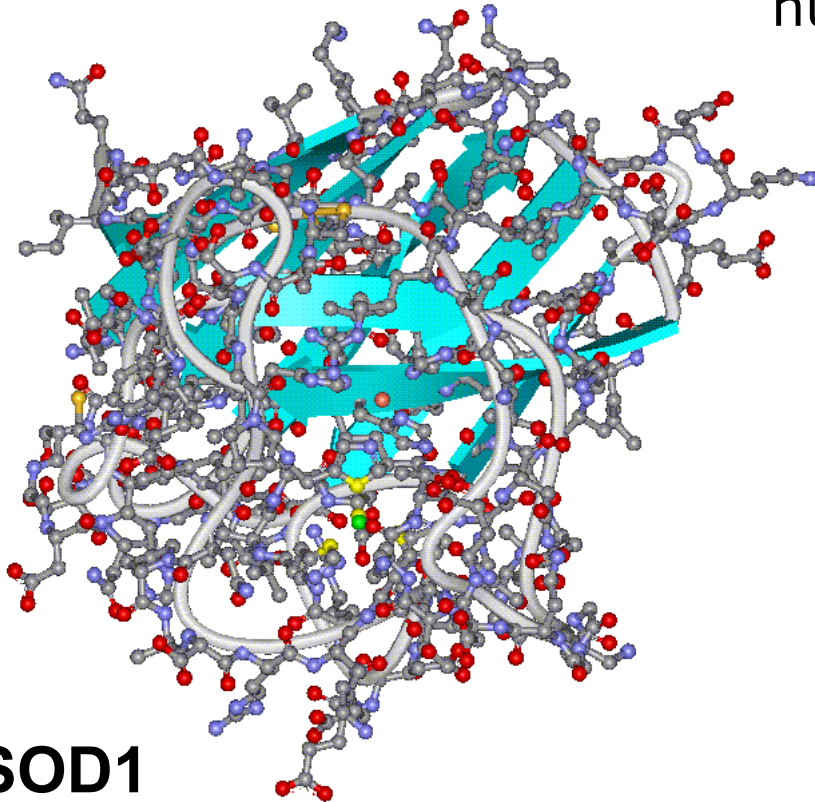
angles 15

harm	1	4	2	71.00000	108.40000
harm	1	4	3	71.00000	108.40000
harm	1	4	9	92.20000	111.30000
harm	2	4	3	71.00000	108.40000
harm	2	4	9	92.20000	111.30000
harm	3	4	9	92.20000	111.30000
harm	5	8	6	71.00000	108.40000
harm	5	8	7	71.00000	108.40000
harm	5	8	9	92.20000	111.30000
harm	6	8	7	71.00000	108.40000
harm	6	8	9	92.20000	111.30000
harm	7	8	9	92.20000	111.30000
harm	4	9	8	68.00000	95.00000
harm	4	9	10	158.00000	106.75000
harm	8	9	10	158.00000	106.75000

Also 12 dihedrals, and 10 vdw (CHARMM)

How about this?

Protein molecules consist of
hundreds of amino acids.



CHARMM22 FF
4382 atoms (exclude water)
19400 two-body
7993 three-body
13000 four body
730 vdw

Clearly, manual entry is not practical



DL_FIELD – helps you to set up force field models.