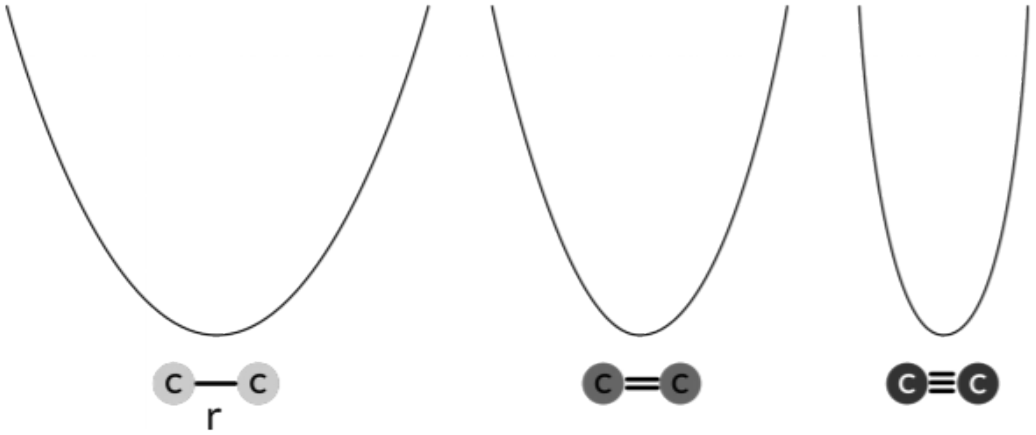
Intro Force Fields (FF)

A FF provides potential energy, E(x), for a given molecular structure (x) via parametrized, analytical functions

$$E_{FF} = E_{bond} + E_{angle} + E_{dihedral} + E_{electrostatic} + E_{v.d.Waals}$$

Example

Bonding energy via harmonic potentials $E_{bond} = k\,(r-r_{eq})^2$



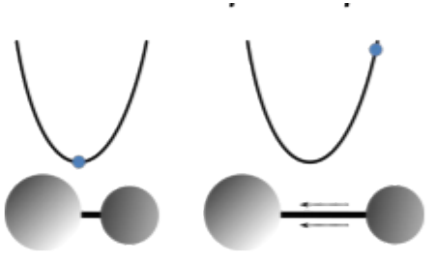
Parameters: k, r_{eq} per atomtype

Atomtypes: C ≠ C ≠ C

(CC_{single}, CC_{double}, CO_{single}, CO_{double}, etc...)

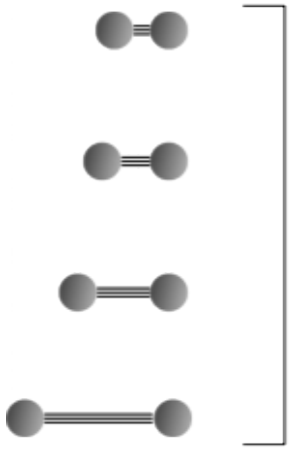
Classical Force Fields vs. ReaxFF

Classical Force Fields



Fixed atomtypes and harmonic potentials:
bond breaking impossible, e.g.

$E_{bond} \propto (distance)^2$

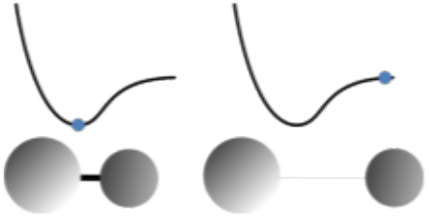


-a triple "bond" will always stay a triple "bond"

- a C_{triple} atom will always be a C_{triple} atom

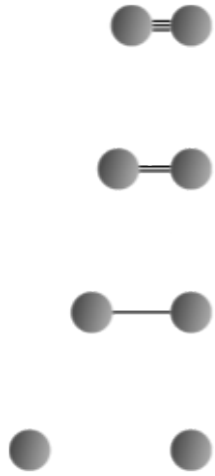
($E_{bond} \rightarrow \infty$)

ReaxFF (Reactive Force Field)

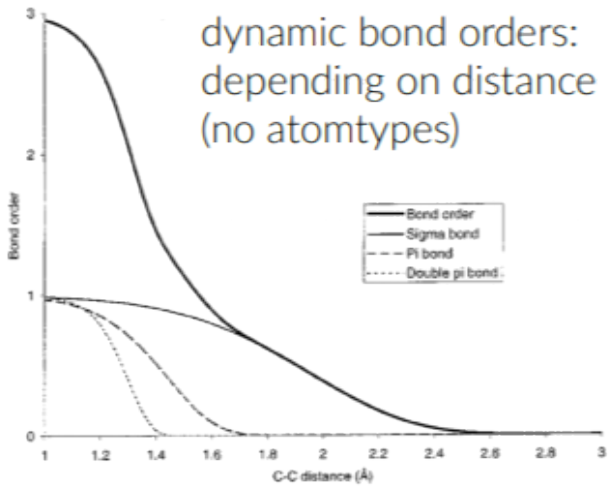


Non-harmonic potentials based on bond orders:
bond breaking/forming possible, e.g.

$E_{bond} \propto -(bond\ order) \times \exp[\ (1 - bond\ order)\ ]$



dynamic bond orders:
depending on distance
(no atomtypes)

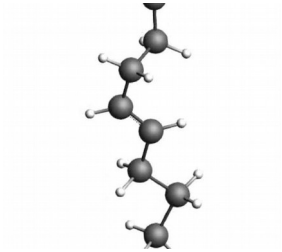


($E_{bond} \rightarrow 0$)

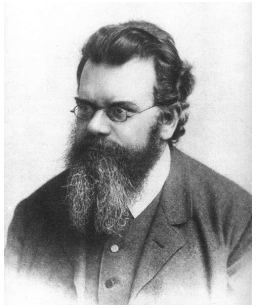
A.C.T. van Duin *et al.J. Phys. Chem. A* 2001, 105, 9396-9409.

Intro to Molecular Dynamics (MD)

What is simulated?
Simulate movement of atoms



Why?
Predict many properties, e.g.
- Thermodynamics
- Kinetics
- Mechanical properties
- much more...



Ludwig Boltzmann
Founded *statistical mechanics* which allow us to explain macroscopic behaviour from ensembles of microscopic entities.

How?
By numerically solving
Newton's equation of motion

$$F = ma = m\left(\frac{d^2x}{dt^2}\right) \qquad F = -\left(\frac{dV}{dx}\right)$$

e.g. with classic Verlet algorithm

$$x_{i+1} = 2\,x_i - x_{i-1} + \frac{(\Delta t)^2}{m} F_i$$

$x_i : Current\ position$

$x_{i-1} : Previous\ position$

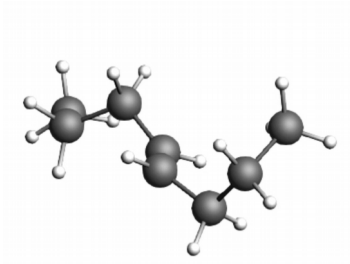
$x_{i+1} : Future\ position$

$\Delta t : Time\ step\ (t_{i+1} - t_i)$

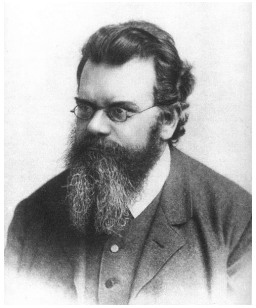
$F_i : Force\ acting\ on\ particle\ at\ position\ x_i$

Intro to Molecular Dynamics (MD)

What is simulated?
Simulate movement of atoms



Why?
Predict many properties, e.g.
- Thermodynamics
- Kinetics
- Mechanical properties
- much more...



Ludwig Boltzmann
Founded *statistical mechanics* which allow us to explain macroscopic behaviour from ensembles of microscopic entities.

How?
By numerically solving
Newton's equation of motion

$$F = ma = m\left(\frac{d^2x}{dt^2}\right) \qquad F = -\left(\frac{dV}{dx}\right)$$

e.g. with classic Verlet algorithm

$$x_{i+1} = 2x_i - x_{i-1} + \frac{(\Delta t)^2}{m} F_i$$

User input

x_i : *Current position*

x_{i-1} : *Previous position*

x_{i+1} : *Future position*

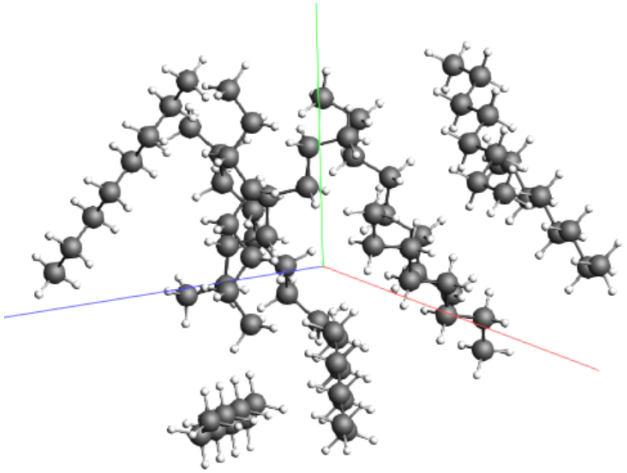
AMS engine (e.g. ReaxFF)

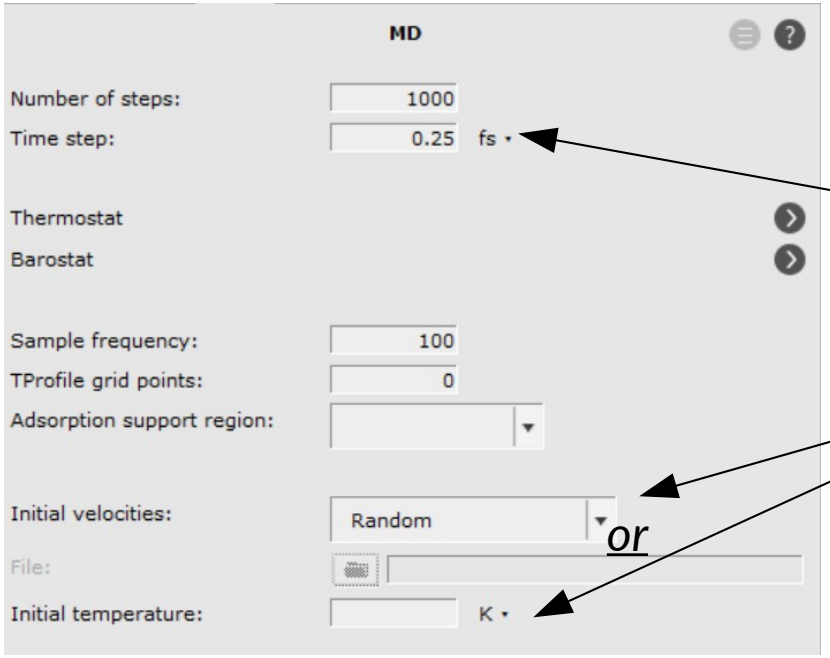
Δt : *Time step* $(t_{i+1} - t_i)$

F_i : *Force acting on particle at position* x_i

MD simulations require initial conditions to start.

Minimal MD setup





How?

By numerically solving
Newton's equation of motion

$$F = ma = m\left(\frac{d^2x}{dt^2}\right) \qquad F = -\left(\frac{dV}{dx}\right)$$

e.g. with classic Verlet algorithm

$$x_{i+1} = 2x_i - x_{i-1} + \frac{(\Delta t)^2}{m} F_i$$

x_i : *Current position*

Δt : *Time step* $(t_{i+1} - t_i)$

x_{i+1} : *Future position*

x_{i-1} : *Previous position*

F_i : *Force acting on particle at position* x_i

Demo