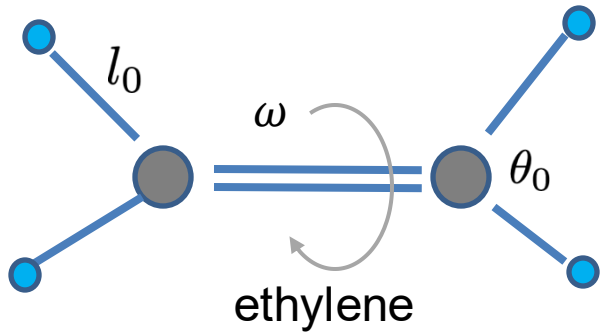
Generalized interatomic potential

$$U = \sum_{bond} \frac{k}{2}(l_i - l_0)^2 + \sum_{angle} \frac{g}{2}(\theta_i - \theta_0)^2 + \sum_{torsion} \frac{v}{2}(1+\cos(n\omega - \gamma)) + \sum_i \sum_{j \neq i} \left\{ 4\epsilon \left[\left(\frac{r_m}{r} \right)^{12} - \left(\frac{r_m}{r} \right)^{6} \right] + \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r} \right\}$$

Bond length Bond angle Bond twisting interatomic coulombic

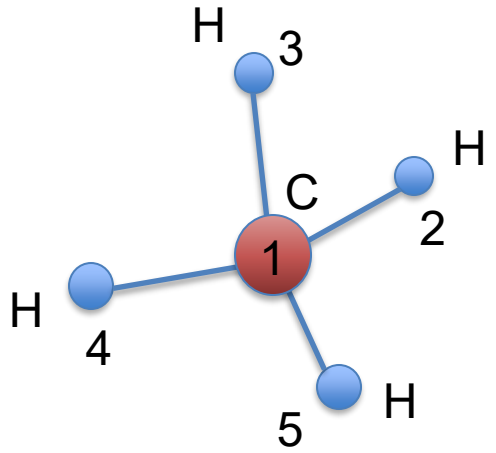
- Metallic bond: Lennard-Jones should be good.
- Ionic bond: add coulombic interaction
- Covalent bond: add bond length, bond angle, bond twist
- The first 3 terms in the equation above indicate that stretch bond length, change bond angle, twist bond plane all cost energy. The equilibrium bonds will stay at l_0 length, θ_0 angle, and a give twist angle γ.



Example initial data file

```
LAMMPS data file for a single CH4 molecule

5 atoms
4 bonds
6 angles

2 atom types
1 bond types
1 angle types

-5.0 5.0 xlo xhi
-5.0 5.0 ylo yhi
-5.0 5.0 zlo zhi

Masses

1 12.011 # Carbon
2 1.008 # Hydrogen

Atoms

1 1 1 0.0 0.0 0.0 0.0 # C (atom_id molecule_id atom_type charge x y z)
2 1 2 0.0 0.0 0.0 1.09 # H
3 1 2 0.0 1.028 -0.37 0.65 # H
4 1 2 0.0 -0.65 0.94 -0.37 # H
5 1 2 0.0 -0.37 -0.65 -0.94 # H
```

```
Bonds

1 1 1 2 # bond_id bond_type atom1 atom2
2 1 1 3
3 1 1 4
4 1 1 5

Angles

1 1 2 1 3 # angle_id angle_type atom1 atom2 atom3 (atom2 is central)
2 1 2 1 4
3 1 2 1 5
4 1 3 1 4
5 1 3 1 5
6 1 4 1 5
```



Example LAMMPS input file


```
# LAMMPS input script for a single CH4 molecule

# 1. Initialization
units real
atom_style full # Use 'full' for charges, bonds, angles, dihedrals
boundary p p p # Periodic boundaries in all directions

# 2. Atom and molecule definition
read_data CH4_01.lmp # Read atom types, coordinates, bonds, etc. from a data file

# 3. Force Field Parameters
pair_style lj/cut 10.0
pair_coeff 1 1 0.100 3.55 # C-C parameters (example)
pair_coeff 2 2 0.030 2.50 # H-H parameters (example)
pair_coeff 1 2 0.050 3.00 # C-H parameters (example)

bond_style harmonic
bond_coeff 1 350.0 1.09 # C-H bond (force constant, equilibrium distance)

angle_style harmonic
angle_coeff 1 50.0 109.5 # H-C-H angle (force constant, equilibrium angle)

# 4. Simulation Settings
neighbor 2.0 bin
neigh_modify delay 0 every 1 check yes

# 5. Minimization (optional)
minimize 1.0e-4 1.0e-6 1000 10000

# 6. Simulation Ensemble (e.g., NVT)
fix 1 all nvt temp 300.0 300.0 100.0 # NVT ensemble at 300K, damping 100fs

# 7. Output
thermo 100
thermo_style custom step temp pe ke etotal press vol lx ly lz
dump 1 all atom 100 dump.lammpstrj # Dump trajectory every 100 steps

# 8. Run
run 10000 # Run for 10,000 timesteps
```

Initial data of atoms

Lennard-Jones

Bond length

Bond angle

Molecular dynamics simulations

Advantages:

- Relatively simple, only use the classical mechanics
- Can calculate many thermodynamic & kinetic quantities

Disadvantages:

- Very small system, in space
- Extremely short physical time
- Rely on accurate interatomic potential (not often available)

New techniques:

- Ab initio MD: Combine PDE solving and Newton's law: Use DFT (solve Schrotinger Eq) to calculate inter-atomic potential, which is then used in Newton's law for atom motion.
- Machine learned inter-atomic potential (MLIP) → Use neutral network to fit DFT results to construct interatomic potentials.

Open-source MD simulation package.
https://www.lammps.org
https://github.com/lammps/lammps

Only need to create initial atomic positions and write an input file to designate simulation conditions.

NIST Interatomic Potentials Repository
https://www.ctcms.nist.gov/potentials/

You can find many interatomic potentials there.

There are many other tools, such as Ovito, for visualization of MD results.