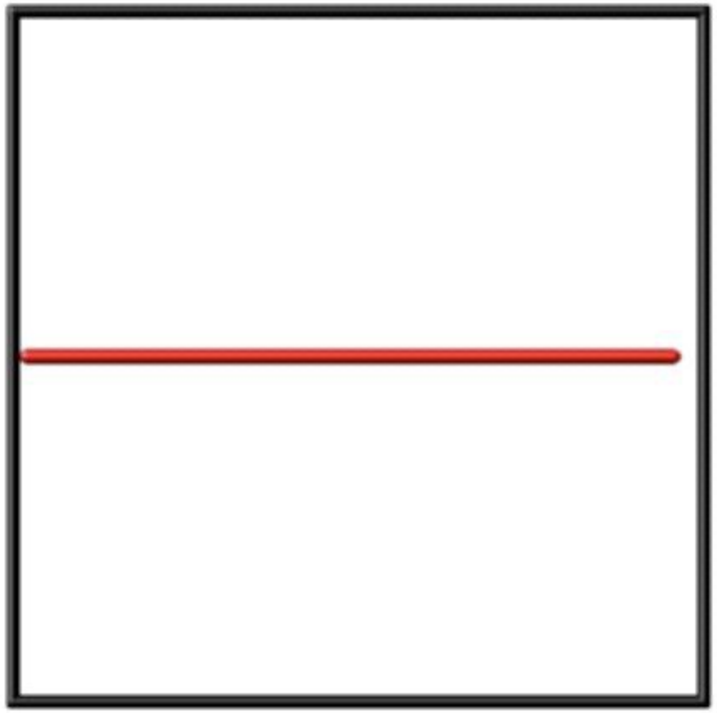
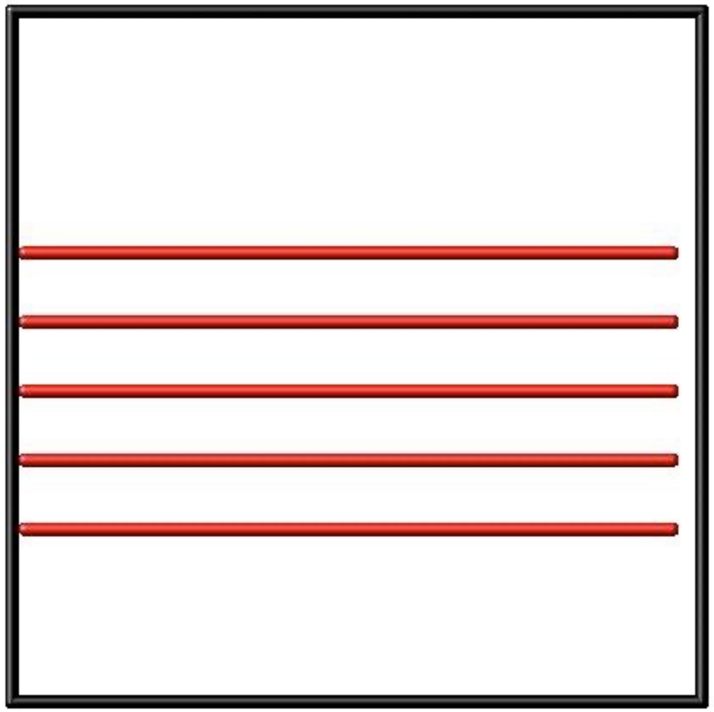
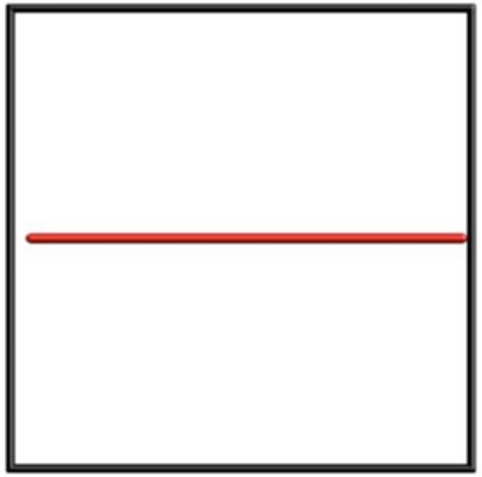
Single and multiple polymer simulations





Single and multiple polymer simulations



```
pair_style          lj/cut 1.12246204830937
pair_coeff          * * 1.0 1.0 1.12246204830937
```

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c$$

ϵ (energy units)

σ (distance units)

LJ cutoff (distance units)

```
#FENE type bond =
```

to define a finite extensible nonlinear elastic (FENE) potential , used for bead-spring polymer models

```
bond_style fene
bond_coeff 1 30.0 1.5 1.0 1.0
special_bonds fene
```

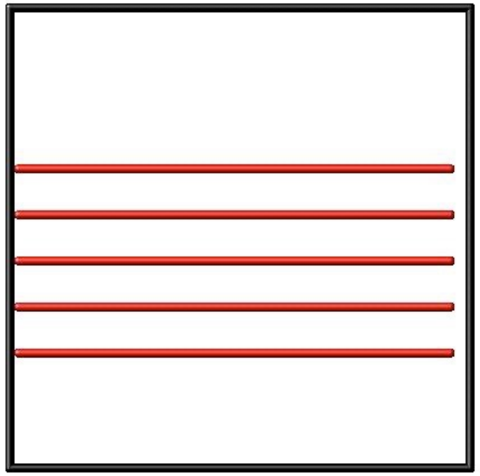
$$E = -0.5KR_0^2 \ln\left[1 - \left(\frac{r}{R_0}\right)^2\right] + 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \epsilon$$

K (energy/distance^2)

R_0 (distance)

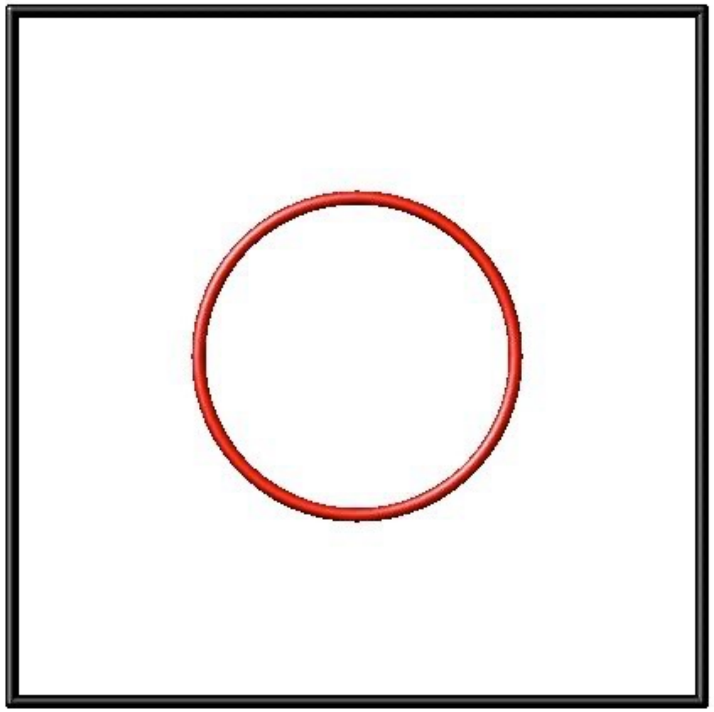
ϵ (energy)

σ (distance)

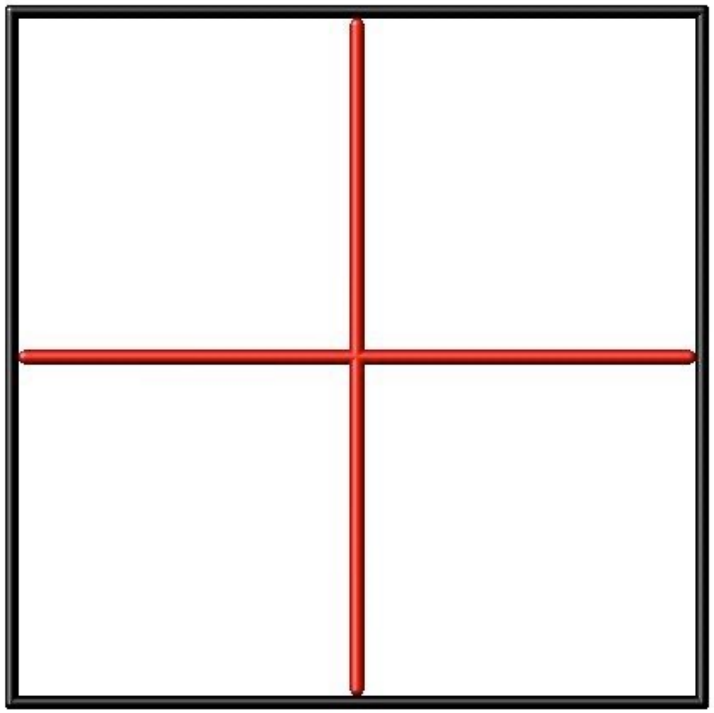


```
atom_style molecular
```

Circular polymer

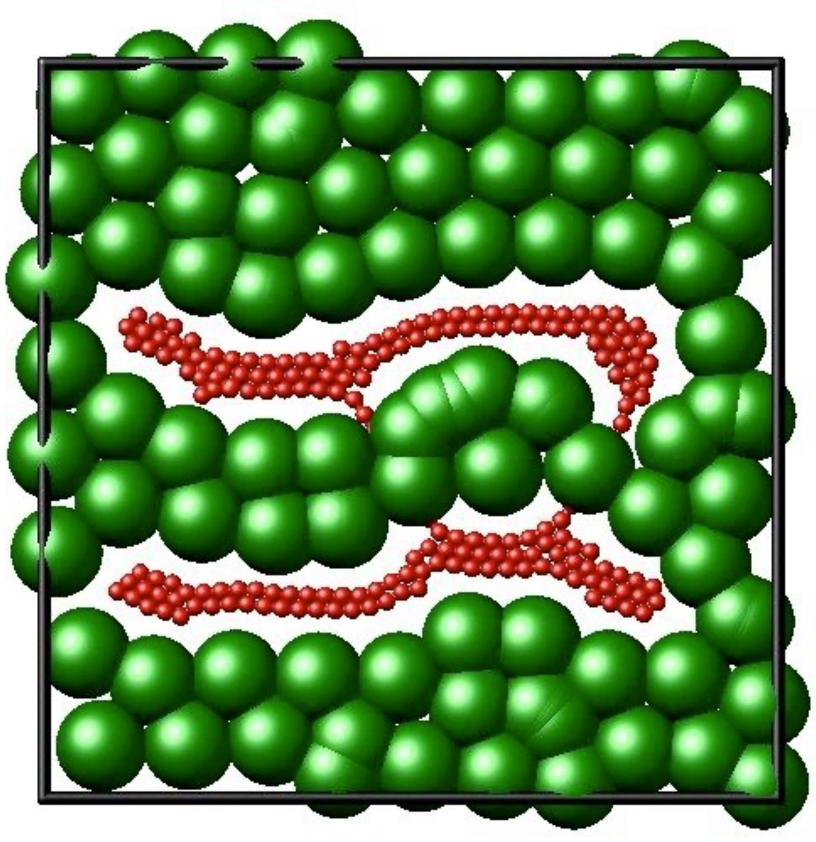


Cross-shaped polymer

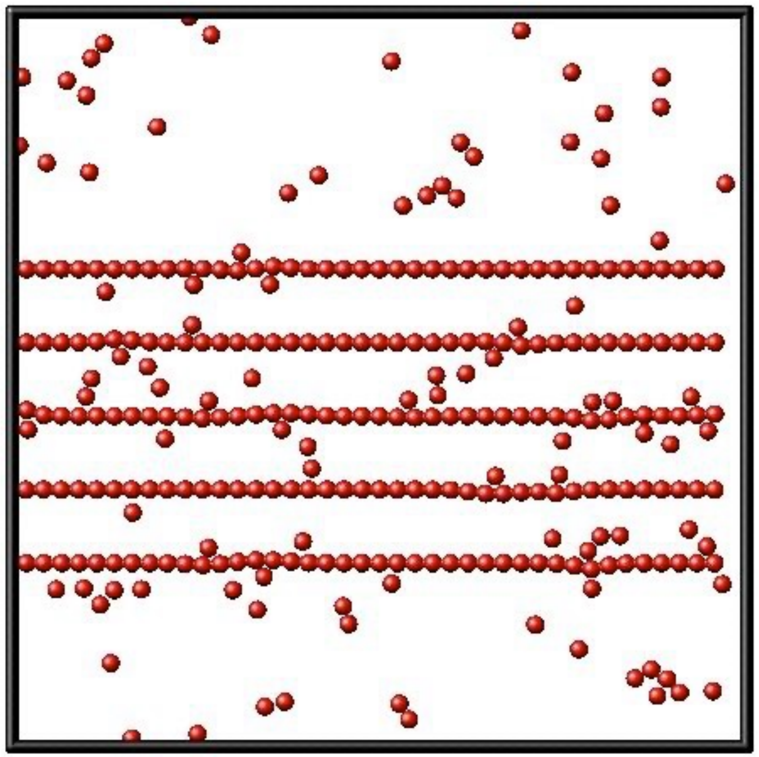


Putting it all together

Polymers with solvent

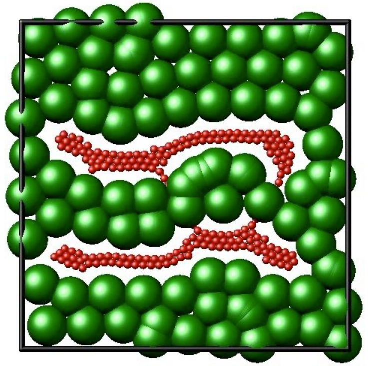


400 particles
Type 2

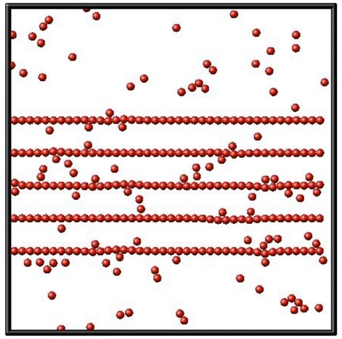


100 particles
Type 2

Polymers with solvent



400 particles
Type 2



100 particles
Type 2

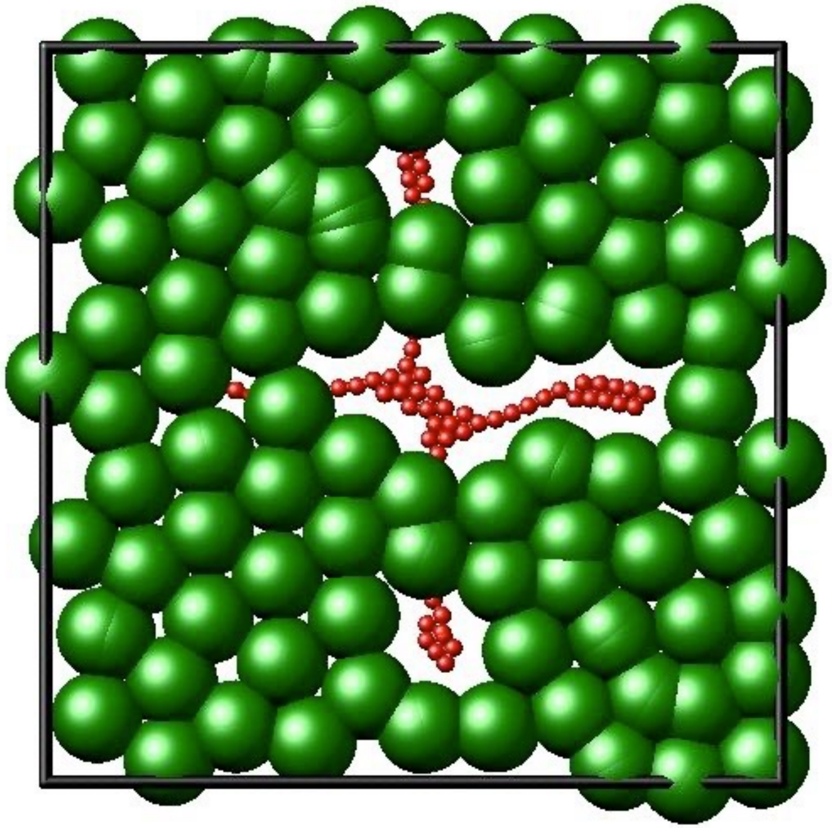
```
pair_style soft       1.0
pair_coeff 1 1 10.0  1.0
pair_coeff 1 2 10.0  5.0
pair_coeff 2 2 10.0  5.0
```

$$E = A\left[1 + \cos\left(\frac{\pi r}{r_c}\right)\right] \qquad r < r_c$$

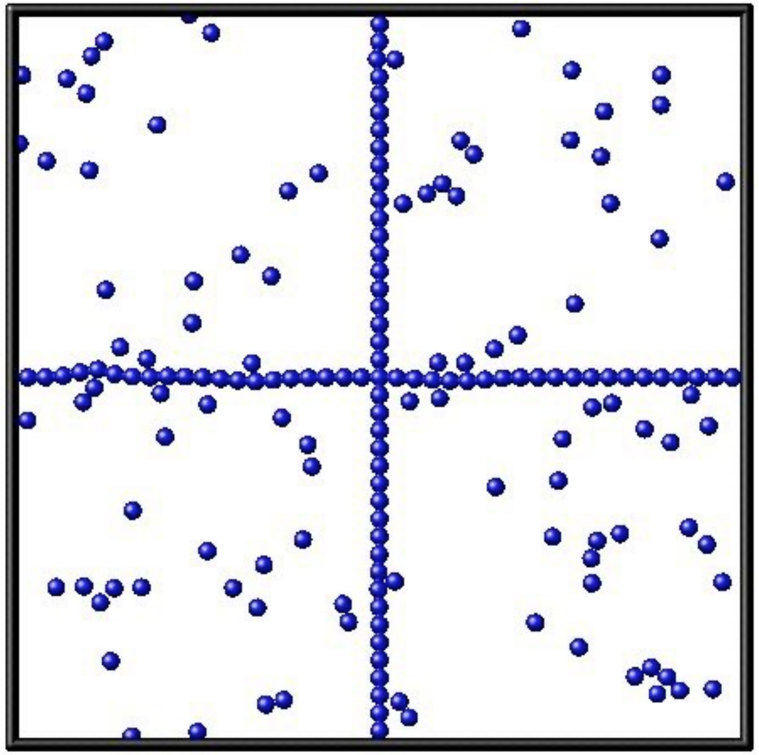
A (energy units)

cutoff (distance units)

Star polymer with particles

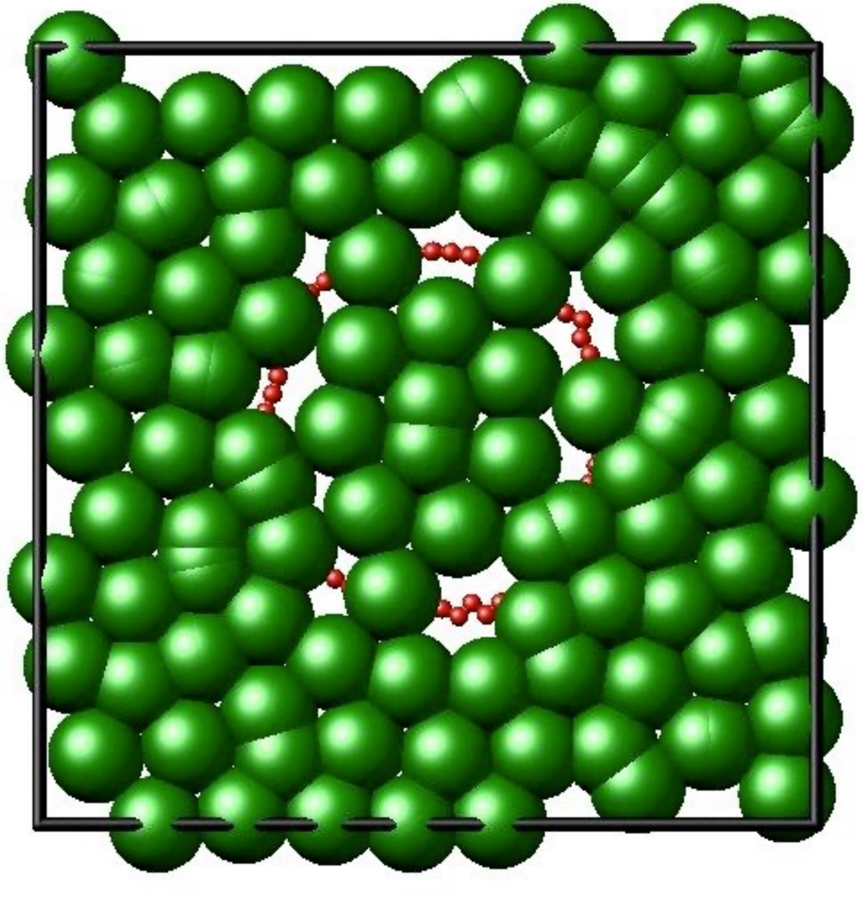


400 particles
Type 2

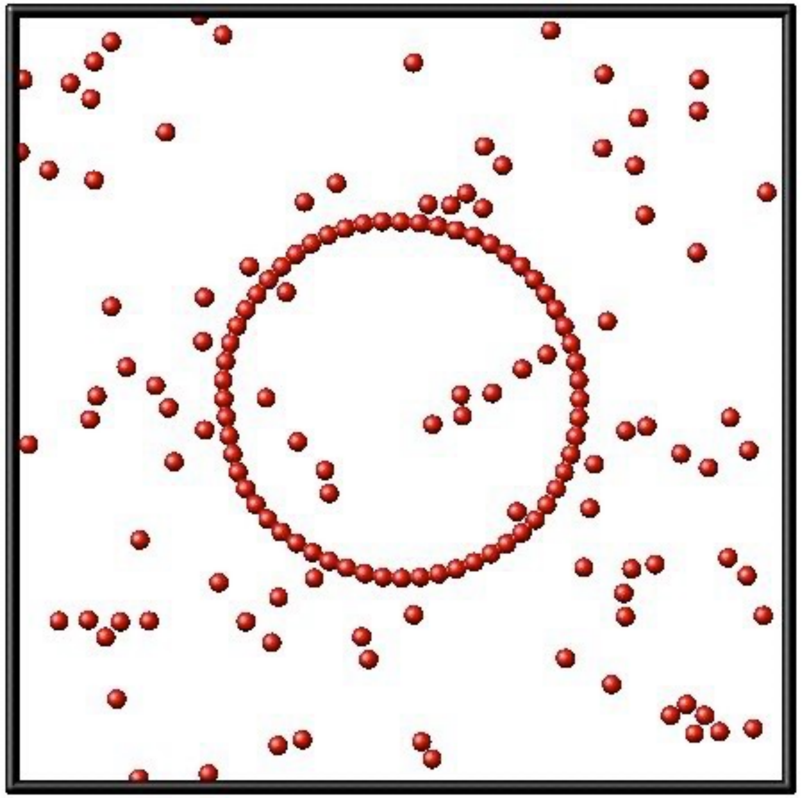


100 particles
Type 2

Circular polymer with particles



400 particles
Type 2



100 particles
Type 2

Future Plans

- Incorporate Martini Model
- Establish a bilayer membrane
- Insert membrane protein from RCSB Protein data bank
- Study Radius of gyration in response to changes in environment or biological structures such as membrane
    - pH and charge differences