COPSS: Force field

1. Particle - particle force types

Particle-particle force types defines the force types between particle and particles.

> ```
> particle_particle_force_types = 'pp_ev_gaussian,
> pp_ev_gaussian_polymerChain, ...'
> pp_ev_gaussian = 'param1, param2, ...'
> pp_ev_gaussian_polymerChain = 'param1, param2, ...'
> ```

Supposing that we have two particles i and j, located at R_i and R_j and the forces on which are f_i and f_j respectively.

$\vec{f}_{ij}$: force acting on particle i by particle j.
$\vec{R}_{ij}$: vector pointing from i to j , i.e., $\vec{R}_{ij} = \vec{R}_j - \vec{R}_i$, which is automatically updated due to periodic boundary conditions.
$\vec{r}_{ij}$: unit vector of $\vec{R}_{ij}$
R_{size}: length of $\vec{R}_{ij}$, i.e., $\vec{R}_{ij} = R_{size} * \vec{r}_{ij}$
a: bead radius. All lengths are non-dimensionalized by this length.
b_k: Kuhn length
$N_{k,s}$: number of Kuhn length per spring
q_0: maximum spring length, $q_0 = N_{k,s} * b_k$
L: contour length of the DNA molecule, $L = N_s * q_0$
S_s^2: radius of gyration of an ideal chain consisting of $N_{k,s}$ Kuhn segments, $S_s^2 = N_{k,s} * b_k^2/6$

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pp_ev_gaussian

> pp_ev_gaussian = ‘c_1, c_2’

pp_ev_gaussian defines a gaussian potential between point particles (**beads only**), two nondimensional parameters need to be given for this force type, c_1 (energy) and c_2 (length).

Then this gaussian force:

> $$\vec{f}_{ij} = -c_1 * c_2 * e^{-c_2 * R^2_{size}} * \vec{r}_{ij}$$
> $$\vec{f}_i += \vec{f}_{ij}$$

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pp_ev_gaussian_polymerChain

> pp_ev_gaussian_polymerChain = ‘ev’

pp_ev_gaussian_polymerChain defines a gaussian potential between beads of worm-like polymer chain **(polymer chain only)**, the only required parameter ev is the nondimensional excluded volume of beads. The coefficient of this gaussian potential is set by default as:

> $$c_1 = ev * a^3 * N^2_{k,s} * (\frac{3.}{4. * \pi * S^2_s})^{3/2}$$
> $$c_2 = 3. * \frac{a^2}{4. * S^2_s}$$

Then this gaussian force:

> $$\vec{f}_{ij} = -c_1 * c_2 * e^{-c_2 * R^2_{size}} * \vec{r}_{ij}$$
> $$\vec{f}_i += \vec{f}_{ij}$$

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pp_ev_lj_cut

> pp_ev_lj_cut = ‘ϵ, σ, r_{cut}’

pp_ev_lj_cut defines a Lennard-Jones potential between two particle i and j. Three non-dimensional parameters, ϵ (energy), σ (particle diameter or slighter bigger, e.g., 2.1), r_{cut} (cutoff radius) are required for this force field.

Then the lj force:

> if $R_{size} <= r_{cut}$:
> $\vec{f}_{ij} = -24 * \epsilon * (2 * (\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6})$
> $\vec{f}_i += \vec{f}_{ij}$
> else:
> $\vec{f}_i += \vec{0}$

pp_ev_lj_repulsive

> pp_ev_lj_repulsive = 'ϵ, σ'

pp_ev_lj_repulsive defines a repulsive Lennard-Jones potential between two particle i and j. Two non-dimensional parameters, ϵ (energy), σ (particle diameter or slighter bigger, e.g., 2.1) are required for this force field.

r_{cut} is set to be the equilibrium length where lj force is zero:

> $r_{cut} = 2^{\frac{1.}{6.}} * \sigma$

Then the repulsive lj force:

> if $R_{size} <= r_{cut}$:
> $\vec{f}_{ij} = -24 * \epsilon * (2 * (\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6})$
> $\vec{f}_i += \vec{f}_{ij}$
> else:
> $\vec{f}_i += \vec{0}$

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pp_ev_harmonic_repulsive

> pp_ev_harmonic_repulsive = 'k, r_0'

pp_ev_harmonic_repulsive defined a repulsive harmonic potential between particle i and j. Two non-dimensional parameters, k(energy) and r_0 (equilibrium length) are required for this force field.
Then the repulsive harmonic force:

> if $R_{size} < r_0$:
> $\vec{f}_{ij} = k * (R_{size} - r_0) * \vec{r}_{ij}$
> $\vec{f}_i + = \vec{f}_{ij}$
> else :
> $\vec{f}_i + = \vec{0}$

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pp_wormLike_spring

> pp_wormLike_spring

pp_wormLike_spring defines spring forces for worm-like bead spring chains (**polymer chain only**). All parameters are set by default in COPSS.

> $c_1 = \frac{a}{2*b_k}$
> $L_s = \frac{N_{k,s}*b_k}{a}$

Then the spring force:

> $\vec{f}_{ij} = c_1 * ((1 - \frac{R_{size}}{L_s})^{-2} - 1. + 4 * \frac{R_{size}}{Ls}) * \vec{r}_{ij}$
> $= \frac{a}{2*b_k}((1 - \frac{R_{size}}{N_{k,s}*b_k/a})^{-2} - 1. + 4 * \frac{R_{size}}{N_{k,s}*b_k/a}) * \vec{r}_{ij}$
>
> $\vec{f}_i + = \vec{f}_{ij}$

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p_constant

> p_constant = ‘f_x, f_y, f_z’

p_constant defines a constant force field on all of the beads. Three parameters (force on x, y, z), f_x, f_y, f_z are needed for the force field.
Then the constant force:

> $\vec{f}_{constant} = (f_x, f_y, f_z)$
> $\vec{f}_i += \vec{f}_{constant}$

2. Particle - wall force types

Particle-wall force types defines the force types between particles and wall, which has to be neither periodic boundary and inlet/outlet.

```
particle_wall_force_types = 'pw_ev_empirical_polymerChain,
pw_ev_lj_cut, ...'
pw_ev_empirical_polymerChain = 'param1, param2, ...'
pw_ev_lj_cut = 'param1, param2, ...'
```

Wall type can only be either **slit** or **sphere** for now, and will be extended to more types in further development. Supposing that we have particle i, located at R_i and the forces on which is f_i.

$\vec{f}_{iw}$: force acting on particle i by wall.
$\vec{R}_{iw}$: vector pointing from i to wall.

> **if wall_type = ‘slit’** : $\vec{R}_{i,lo} = \overrightarrow{box_{min}} - \vec{R}_i, \vec{R}_{i,hi} = \overrightarrow{box_{max}} - \vec{R}_i$ And we need to compute particle-wall interaction for lower wall and upper wall separately.
> **if wall_type = ‘sphere’** : $\vec{R}_{iw} = \vec{r}_i * (R_{sphere} - |\vec{R}_i|)$, where $\vec{r}_i$ is the unit vector of $\vec{R}_i$, $|\vec{R}_i|$ is the distance of particle i to origin.

$\vec{r}_{iw}$: unit vector of $\vec{R}_{iw}$.
R_{size}: length of $\vec{R}_{iw}$, i.e., $\vec{R}_{iw} = \vec{r}_{iw} * R_{size}$

pw_ev_empirical_polymerChain

> pw_ev_empirical_polymerChain

pw_ev_empirical_polymerChain defines an empirical bead_wall repulsive potential on polymer beads (**polymer chain only**). All parameters are set by default in COPSS:

> $c_1 = a/b_k$
> $c2 = c1/\sqrt{N_{k,s}} = \frac{a}{b_k * \sqrt{N_{k,s}}}$
> $d_0 = 0.5/c_2 = \frac{b_k * \sqrt{N_{k,s}}}{2 * a}$
> $c_0 = 25 * c_1 = \frac{25 * a}{b_k}$

Then the empirical force:

> **if** $R_{size} < d_0$:
> $\vec{f}_{iw} = -c_0 * (1 - \frac{R_{size}}{d_0})^2 * \vec{r}_{iw}$
> $= -\frac{25 * a}{b_k}(1 - \frac{2 * R_{size} * a}{b_k * \sqrt{N_{k,s}}})^2 * \vec{r}_{iw}$
> $\vec{f}_i += \vec{f}_{iw}$
> **else** :
> $\vec{f}_i += 0$

The corresponding potential is:

> **if** $R_{size} < d_0$:
> $U_i^{wall} = \frac{A_{wall}}{3 * b_k / a * d_0}(R_{size} - d_0)^3$, where $A_{wall} = 25/a$
> **else**:
> $U_i^{wall} = 0$

---

pw_ev_lj_cut

> pw_ev_lj_cut = 'ϵ, σ, r_{cut}'

pw_ev_lj_cut defines a Lennard-Jones potential between particle i and the wall. Three non-dimensional parameters, ϵ (energy), σ (particle radius or slighter bigger, e.g., 1.05), r_{cut} (cutoff radius) are required for this force field.

Then the lj force:

> if $R_{size} <= r_{cut}$:
> $\vec{f}_{iw} = -24 * \epsilon * (2 * (\frac{\sigma}{r_{iw}})^{12} - (\frac{\sigma}{r_{iw}})^{6})$
> $\vec{f}_{i} += \vec{f}_{iw}$
> else:
> $\vec{f}_{i} += \vec{0}$

---

pw_ev_lj_repulsive

> pw_ev_lj_repulsive = 'ϵ, σ'

pw_ev_lj_repulsive defines a repulsive Lennard-Jones potential between particle i and the wall. Two non-dimensional parameters, ϵ (energy), σ (particle radius or slighter bigger, e.g., 1.05) are required for this force field.

r_{cut} is set to be the equilibrium length where lj force is zero:

> $r_{cut} = 2^{\frac{1.}{6.}} * \sigma$

Then the repulsive lj force:

> if $R_{size} <= r_{cut}$:
> $\vec{f}_{iw} = -24 * \epsilon * (2 * (\frac{\sigma}{r_{iw}})^{12} - (\frac{\sigma}{r_{iw}})^{6})$
> $\vec{f}_{i} += \vec{f}_{iw}$
> else:
> $\vec{f}_{i} += \vec{0}$

---

pw_ev_harmonic_repulsive

> pw_ev_harmonic_repulsive = ‘k, r_0’

pw_ev_harmonic_repulsive defined a repulsive harmonic potential between particle i and the wall. Two non-dimensional parameters, k(energy) and r_0 (equilibrium length, e.g., 1.1) are required for this force field.
Then the repulsive harmonic force:

> if $R_{size} < r_0$:
> $\vec{f}_{iw} = k * (R_{size} - r_0) * \vec{r}_{iw}$
> $\vec{f}_i += \vec{f}_{iw}$
> else :
> $\vec{f}_i += \vec{0}$