The Buckingham-Coulomb potential

From GPUMD
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Brief descriptions

- This is the Buckingham-Coulomb potential, which is also usually referred to as the rigid-ion potential.
- It currently only applies to systems with two atom types.
- The Coulomb potential is treated using the damped-shifted-force (DSF) method as proposed in [Fennell 2006].

Potential form

- It consists of the Buckingham potential

$$U_{ij} = A_{ij} \exp(-b_{ij} r_{ij}) - \frac{C_{ij}}{r_{ij}^6}$$

and a Coulomb potential.

- The Coulomb potential is evaluated using the damped-shifted-force (DSF) method [1]. The DSF version of the pairwise Coulomb potential can be written as:

$$U_{ij} = \frac{q_i q_j}{4\pi\epsilon_0} \left[\frac{\mathrm{erfc}(\alpha r_{ij})}{r_{ij}} - \frac{\mathrm{erfc}(\alpha R_c)}{R_c} + \left(\frac{\mathrm{erfc}(\alpha R_c)}{R_c^2} + \frac{2\alpha}{\sqrt{\pi}} \frac{\exp(-\alpha^2 R_c^2)}{R_c} \right) (r_{ij} - R_c) \right],$$

where **erfc** is the complementary error function.

Parameters

Parameter	Units
A_{ij}	eV
b_{ij}	A^{-1}
C_{ij}	A^6
q_i	e
α	A^{-1}
R_c	A

- α is the electrostatic damping factor and R_c is the cutoff radius for the Coulomb potential.
- In GPUMD, we have fixed α to 0.2 A^{-1}, which is a good choice according to the results in [Fennell 2006].

Potential file

Currently, this potential only applies to systems with two atom types in GPUMD. The potential file for this potential model reads

```
ri 2
q_0   q_1  cutoff
A_00, b_00 C_00
A_11, b_11 C_11
A_01, b_01 C_01
```

References

- [Fennell 2006] Christopher J. Fennell and J. Daniel Gezelter, *Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics* (https://doi.org/10.1063/1.2206581), J. Chem. Phys. **124**, 234104 (2006).