

Constructing Embedded Atom Model (EAM) potential file for LAMMPS

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Abstract

This document presents the anatomy of an EAM potential file for modelling the behaviour of binary iron-helium (Fe-He) system via molecular dynamics (MD) simulation using LAMMPS [1]. The potentials discussed in this document are the Ackland-04, the Aziz-95 and the Gao-11 potentials, describing the Fe-Fe, He-He, and Fe-He interaction, respectively. While the emphasis here is placed upon these potentials, this document can still be used as a guide for constructing a LAMMPS-compatible potential file for EAM binary systems from the literature (Section 3).

1 Background

The iron-helium (Fe-He) system is a binary system. To simulate the behaviour of such system using MD simulations, one needs to employ an interatomic potential that consists of three components: the Fe-Fe, the He-He and the Fe-He interaction. The literature provides few choices for each component; these choices, however, are not independent of each other. For the purpose of my research, I have chosen the following potentials:

1. The Ackland-04 Fe-Fe potential [2].
2. The Gao-11 Fe-He potential [3].
3. The Aziz-05 He-He potential [4].

The potentials in the list above have been selected based on the choice of the Fe-He interaction since this interaction governs the behaviour of helium and grain boundaries in iron. A detailed survey on other options for Fe-He potentials available in the literature can be found in Chapter 4 of my thesis.

The first two components, i.e. the Ackland-04 and the Gao-11 potentials, fall under the type of Embedded Atom Model (EAM) potentials, which express the potential energy as the sum of two-body (pairwise) repulsive interaction between a given atom and its neighbours within a cutoff distance, and many-body attractive interaction that accounts for the contribution from a larger group of neighbouring atoms to the electron density of a given atom. The last component (the Aziz-95 potential) is a simple two-body Coulombic potential, where only the repulsive interaction among atoms are considered. No attractive term is assigned to the He-He potential since He gas is an ideal gas.

The total potential energy of a molecular dynamics simulation cell which contains N_{Fe} iron atoms and N_{He} helium atoms is given by

$$U_{\text{total}} = U_{\text{Fe:Fe}} + U_{\text{Fe:He}} + U_{\text{He:He}} \quad (1)$$

where $U_{\text{Fe:Fe}}$, $U_{\text{Fe:He}}$ and $U_{\text{He:He}}$ are the contribution of interaction among Fe atoms, between Fe and He atoms, and among He atoms, to the total energy, respectively. A brief description of each of these components is presented as follows.

2 Components of EAM file

2.1 Fe-Fe interaction

The formalism of potential energy due to the interaction among Fe atoms, as suggested by Ackland, et al is [2]

$$U_{\text{Fe:Fe}} = \sum_{i=1}^{N_{\text{Fe}}-1} \sum_{j=i+1}^{N_{\text{Fe}}} U_{\text{rep,Fe:Fe}}(r_{ij}) + \sum_{i=1}^{N_{\text{Fe}}} G_{\text{Fe}}(\rho_i) \text{ where } \rho_i = \sum_{j=1}^{N_{\text{Fe}}} \Phi_{\text{Fe},i}(r_{ij}) \quad (2)$$

where r_{ij} is the interatomic distance between Fe atom i and j , $U_{\text{rep,Fe:Fe}}$ is a two-body potential describing the repulsive interaction among two Fe atoms, G_{Fe} is the energy required to embed an Fe atom i into a uniform electron density ρ_i and $\Phi_{\text{Fe},i}$ is the spherically averaged electron density experienced by an Fe atom i due to all of the other Fe atoms in the system.

2.1.1 Repulsive term $U_{\text{rep,Fe:Fe}}$

The repulsive term contains two parts: the short-range screened electrostatic form of Biersack-Ziegler (BZ) [5] and the long-range cubic knot functions (CK). A similar decoupling strategy is also adopted by the Fe-He component, see Section 2.2. In order to connect the two, the Ackland-04 employed a polynomial exponential function. This choice is arbitrary. In the case of Fe-He interaction, Section 2.2, a Fermi-like function is adopted instead of a polynomial exponential function to connect the short-range BZ potential and long-range cubic knots. Before proceeding to the discussion, it is worthwhile to introduce the following notation $H(r - x)$, i.e. a shifted Heaviside function.

$$H(r - x) = \begin{cases} 1 & , \quad x \leq r \\ 0 & , \quad x > r \end{cases} \quad (3)$$

The formalism is given by:

$$U_{\text{rep,Fe:Fe}}(r) = H(r_1 - r) U_{\text{BZ}}(r) + H(r - r_2) U_{\text{CK}} + H(r - r_1) H(r_2 - r) J_c(r) \quad (4)$$

where the description of each term is provided below.

Short-range Biersack-Ziegler (BZ) potential U_{BZ}

The short-range potential U_{BZ} is given by

$$U_{\text{BZ}}(r) = \frac{K_{\text{Fe:Fe}}}{r} \varphi\left(\frac{r}{r_s}\right) \quad (5)$$

where $K_{\text{Fe:Fe}} = \frac{Z_{\text{Fe}} Z_{\text{Fe}} e^2}{4\pi\epsilon_0} \frac{1}{10^{-10}} = 9734.159276 \text{ eV}\cdot\text{\AA}$. Z_1 and Z_2 are the atomic numbers of interacting atom, i.e. $Z_1 = Z_2 = 26$. The distance r is expressed in Ångstrom and scaled by $r_s = 0.4683766 / (Z_1^{2/3} + Z_2^{2/3}) = 0.110693297 \text{ \AA}$. The function $\varphi(x)$ is given by:

$$\begin{aligned} \varphi(x) = & 0.1818 \exp(-3.2x) + 0.5099 \exp(-0.9423x) + \\ & 0.2802 \exp(-0.4029x) + 0.02817 \exp(-0.2016x) \end{aligned} \quad (6)$$

Note that there is an inconsistency between the original form of Biersack-Ziegler potential [5] and the Ackland-04 potential [2] (as well as the preceding Fe-Fe potentials, i.e. the Mendeleev-03 [6] and the Ackland-97 [7] potentials). See Section 2.4 for details.

Long-range Cubic Knot (CK) potential U_{CK}

The long-range potential U_{CK} is given by

$$U_{\text{CK}}(r) = \sum_{k=1}^{13} a_k (r_k - r)^3 H(r_k - r) \quad (7)$$

where coefficients a_k and r_k are given in the following table.

Tab. 1: List of parameters for the cubic knot function in Fe-Fe interaction, Eq. (7) [2]

| k | a_k | r_k | k | a_k | r_k |
|-----|-------------------|-------|-----|---------------------|-------|
| 1 | -27.444805994228 | 2.2 | 8 | -2.3194358924605 | 3.0 |
| 2 | +15.738054058489 | 2.3 | 9 | +2.6577406128280 | 3.3 |
| 3 | +2.2077118733936 | 2.4 | 10 | -1.0260416933564 | 3.7 |
| 4 | -2.4989799053251 | 2.5 | 11 | +0.35018615891957 | 4.2 |
| 5 | +4.2099676494795 | 2.6 | 12 | -0.058531821042271 | 4.7 |
| 6 | -0.77361294129713 | 2.7 | 13 | -0.0030458824556234 | 5.3 |
| 7 | +0.80656414937789 | 2.8 | | | |

Connecting function J_c

The connecting potential has the following form:

$$J_c(r) = \exp(B_0 + B_1 r + B_2 r^2 + B_3 r^3) \quad (8)$$

where the coefficients are given in the following table.

Tab. 2: List of parameters used in the connecting potential [2]

| B_k | value |
|-------|-------------------|
| B_0 | +7.4122709384068 |
| B_1 | -0.64180690713367 |
| B_2 | -2.6043547961722 |
| B_3 | +0.6262539393123 |

2.1.2 Attractive terms $G_{\text{Fe}}, \Phi_{\text{Fe}}$

Electron density Φ_{Fe}

The electron density has the following form:

$$\Phi_{\text{Fe}}(r) = \sum_{k=1}^3 A_k (R_k - r)^3 H(R_k - r) \quad (9)$$

where the coefficients A_k and R_k are given in the following table.

Tab. 3: List of parameters for electron density function of Fe-Fe interaction, Eq. (9) [2]

| k | A_k | R_k |
|-----|-------------------|-------|
| 1 | +11.686859407970 | 2.4 |
| 2 | -0.01471074009883 | 3.2 |
| 3 | +0.47193527075943 | 4.2 |

Embedding function $G_{\text{Fe}}(\rho)$

The embedding function has the following form:

$$G_{\text{Fe}}(\rho) = -\sqrt{\rho} + a_2\rho^2 + a_4\rho^4 \quad (10)$$

where $a_2 = -6.7314115586063 \times 10^{-4}$ and $a_4 = +7.5614905604792 \times 10^{-8}$.

2.2 Fe-He interaction

2.2.1 Repulsive term $U_{\text{rep,Fe:He}}$

Similar to the case of Fe-Fe interaction, the repulsive term contains two parts: the short-range screened electrostatic form of Biersack-Ziegler (BZ) and the long-range cubic knot functions (CK). To connect the two, a Fermi-like function $J_c(r)$ was employed.

The formalism is given by:

$$U_{\text{rep,Fe:He}}(r) = U_{\text{BZ}}(r) [1 - J_c(r)] + U_{\text{CK}}(r) J_c(r) \quad (11)$$

where the description of each term is provided below.

Short-range Biersack-Ziegler (BZ) potential U_{BZ}

Short-range potential U_{BZ} is given by

$$U_{\text{BZ}}(r) = \frac{K_{\text{Fe:He}}}{r} \varphi\left(\frac{r}{r_s}\right) \quad (12)$$

where $K_{\text{Fe:He}} = \frac{Z_{\text{Fe}}Z_{\text{He}}e^2}{4\pi\epsilon_0} \frac{1}{10^{-10}} = 748.7814828 \text{ eV}\cdot\text{\AA}$. Parameter Z_1 and Z_2 are the atomic numbers of interacting atom, i.e. $Z_1 = 26$, $Z_2 = 2$. The distance r is expressed in Ångstrom and scaled by $r_s = 0.4683766 / (Z_1^{0.23} + Z_2^{0.23}) = 0.142429287 \text{ \AA}$. The function $\varphi(x)$ is the same as Eq. (6).

Long-range Cubic Knot (CK) potential U_{CK}

Long-range potential U_{CK} is given by

$$U_{\text{CK}}(r) = \sum_{k=1}^7 a_k (r_k - r)^3 H(r_k - r) \quad (13)$$

where coefficients a_k and r_k are given in the following table.

Tab. 4: List of parameters for cubic knot function in Fe-He interaction, Eq. (13) [3]

| k | a_k | r_k |
|-----|------------------|--------|
| 1 | -45.916354995728 | 1.6155 |
| 2 | 35.550312671661 | 1.6896 |
| 3 | 164.319865173340 | 1.8017 |
| 4 | -1.727464405060 | 2.0482 |
| 5 | 0.106771826237 | 2.3816 |
| 6 | 0.073715269849 | 3.5067 |
| 7 | 0.038235287677 | 3.9028 |

Connecting function J_c

The connecting potential has the following form:

$$J_c(r) = [1 + \exp(-b_f (r - r_f))]^{-1} \quad (14)$$

where $b_f = 10.0 \text{ \AA}^{-1}$ and $r_f = 0.25 \text{ \AA}$.

2.2.2 Attractive terms $F_{\text{He}}, \Phi_{\text{He}}$

Electron density Φ_{He}

The electron density has the following form:

$$\Phi_{\text{He}}(r) = N_s r^3 \exp(-2\xi_s r) H(r_0 - r) \quad (15)$$

where $N_s = 20.0 \text{ \AA}^{-1}$, $\xi_s = 2.8936295071479 \text{ \AA}^{-1}$ and $r_0 = 4.1 \text{ \AA}$.

Embedding function $F_{\text{Fe}}(\rho)$

The embedding function has the following form:

$$F_{\text{Fe}}(\rho) = b_1 \sqrt{\rho} + b_2 \rho^2 + b_3 \rho^4 \quad (16)$$

where coefficients b_1 , b_2 and b_3 are given in the following table.

Tab. 5: List of parameters for embedding function, Eq. (16) [3]

| b_k | value | unit |
|-------|----------------|------------------|
| 1 | 0.220813420485 | eV/Å |
| 2 | 1.367508764130 | eVÅ ⁴ |
| 3 | 3.382256025271 | eVÅ ⁸ |

2.3 He-He interaction

2.3.1 Repulsive term

The Coulombic repulsive potential for He-He interaction is given by[4]:

$$V_{He-He}(r) = \epsilon V^*(x) \quad (17)$$

where

$$V^*(x) = A^* \exp(-\alpha^* x + \beta^* x^2) - G(x) \cdot \left(\frac{c_6}{x^6} + \frac{c_8}{x^8} + \frac{c_{10}}{x^{10}} \right) \quad (18)$$

with

$$G(x) = \begin{cases} \exp\left[-\left(\frac{D}{x} - 1\right)^2\right] & x < D \\ 1 & x \geq D \end{cases} \quad (19)$$

where

$$x = \frac{r}{r_m}$$

The above formalism is actually obtained from [8] via ; reference [4] only listed the model parameters for the formalism above¹. The list of relevant parameters are given in the following table.

¹ Note that ref. [8] discussed about Ar not He. Nevertheless, [4] cited [9] which cited [8].

Tab. 6: List of parameters for the He-He repulsive potential, i.e. Eq. (17-19) [4]

| Parameter | Value | Unit |
|------------|--------------------------|-----------------|
| A^* | 1.86924404×10^5 | [dimensionless] |
| α^* | 10.5717543 | [dimensionless] |
| c_6 | 1.35186623 | [dimensionless] |
| c_8 | 0.41495143 | [dimensionless] |
| c_{10} | 0.17151143 | [dimensionless] |
| β^* | -2.07758779 | [dimensionless] |
| D | 1.438 | [dimensionless] |
| ϵ | 9.441160225 | eV |
| r_m | 2.9683 | Ångstrom |

It is also worth mentioning from [10] that He has a hcp lattice structure with lattice constant of 3.57 Å and atomic mass of 4.002602 amu.

2.3.2 Attractive term

No attractive term is specified by the Aziz-95 potential.

2.4 Note

There is an inconsistency between the original Biersack-Ziegler screening potential [5] and the series of Fe-Fe potentials, i.e. Ackland-04 [2], Mendeleev-03 [6], and Ackland-97 [7]. In the latter group, the power for Z_1 and Z_2 is 2/3, e.g. see the description following Eq. (5). In the original Biersack-Ziegler model, the power for Z_1 and Z_2 is 0.23 [5]. It is unlikely that such a discrepancy is a mere typological error, as evident by the Fe potentials posted on the NIST website:

(<http://www.ctcms.nist.gov/potentials/Fe.html>)

where the power for Z_1 and Z_2 terms is 0.666472. For the purpose of my study, I adopted the power term consistent with that stated in the Fe-Fe potential series, i.e. 0.666472. It is of interest to note that, unlike its Fe-Fe counterpart, the repulsive term for Fe-He potential is consistent with the original Biersack-Ziegler model, see the description following Eq. (12). Additionally, the NIST potentials use an arbitrarily large value of U_{BZ} when r is less than a critical value, i.e. $U_{BZ} = U_{BZ,crit}$ for $r \leq r_{crit}$. These are $(r_{crit}, U_{BZ,crit}) = (0.5 \text{ Å}, 10^{12} \text{ eV} \cdot \text{Å})$.

3 Anatomy of LAMMPS-compatible EAM potential file

The LAMMPS-compatible EAM potential files are written in setfl format, the anatomy of which is described in the following table.

Tab. 7: Line-by-line description of a setfl file

| Line # | Description |
|--|--|
| 1 | A non-value statement. I included citation to [2] here. |
| 2 | A non-value statement. I included citation to [4] here. |
| 3 | A non-value statement. I included citation to [3] here. |
| 4 | (int number_of_elem) (Name of 1st element) (Name of 2nd element) /* Implementation example: 2 Fe He |
| 5 | (int NPTS_RHO) (double RHO_increment) (int NPTS_DIST)↔ (double DIST_increment) (double r_cutoff) /* • NPTS_RHO = number of data points of rho in the file, –e.g. [2] uses 10,000 data points; • RHO_increment = increment of rho–e.g. 0.05; • NPTS_DIST = number of data points for r_distance; • DIST_increment = r_cutoff/NPTS_DIST; • r_cutoff = the greatest max. range of repuls. potential from the 2 elements –e.g. in the case of Fe-He system, r_cutoff is from Fe, i.e. 5.3 Å */ /* Implementation example: 10000 5E-02 10000 5.3E-04 5.3E+00 |
| 6 | (int Z1) (double Ar_Z1) (double lattparam_Z1) (string crystalstruc_Z1) /* • Z1 = atomic number of elem 1; • Ar_Z1 = atomic mass of elem 1; • lattparam_Z1 = lattice parameter of elem 1; • crystal_struc_Z1 = crystal structure of element1 */ /* Implementation example: 26 5.585E+01 2.855312E+00 bcc |
| 7 to (NPTS_RHO/5 + 6) | each line contains 5 values, each value is calculated from the embedded function of element 1. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the electron density of element 1 - element 1. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the electron density of element 1 - element 2. |

| | |
|--|---|
| Cont. from prev. line | <pre>(int Z2) (double Ar_Z2) (double lattparam_Z2) ← (string crystalstruc_Z2) /* • Z2 = atomic number of elem 2; • Ar_Z2 = atomic mass of elem 2, • lattparam_Z2 = lattice parameter of elem 2; • crystal_struc_Z2 = crystal structure of element2 */ /* Implementation example: 2 4.0026E+00 3.570E+00 hcp</pre> |
| Cont. from prev. line until the next (NPTS_RHO/5 - 1) | each line contains 5 values, each value is calculated from the embedded function of element 2. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the electron density of element 1 - element 2. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the electron density of element 2 - element 2. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the REPULSIVE potential of element 1 - element 1. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the REPULSIVE potential of element 1 - element 2. |
| Cont. from prev. line until the next (NPTS_DIST/5 - 1) | each line contains 5 values, each value is calculated from the REPULSIVE potential of element 2 - element 2. |

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