Embedded Atom Method
Energy, Force and Tangent

Sylvie Aubry
Sandia National Laboratories, CA

1 EAM Potential

EAM potential is defined by

$$\mathcal{E} = \sum_i^n \left[E_i^e \left(\sum_j^{n_i} \rho_j(r_{ij}) \right) + \sum_j^{n_i} \frac{[z(r_{ij})]^2}{r_{ij}} \right]$$

E^e is the embedded energy, $\bar{\rho}_i$ is the electron density

$$E^e = \sum_i^n E_i(\bar{\rho}_i) = \sum_i^n E_i \left(\sum_j^{n_i} \rho_j(r_{ij}) \right)$$

and, Φ is a pair potential

$$\Phi = \frac{1}{2} \sum_i^n \sum_j^{n_i} \phi(r_{ij}) = \frac{1}{2} \sum_i^n \sum_j^{n_i} \frac{z_i(r_{ij}) z_j(r_{ij})}{r_{ij}}$$

where n_i are the neighbors of i.

2 EAM Force

Let's note that

$$\phi(r) = \frac{z_i(r) z_j(r)}{r}$$

and,

$$\phi'(r) = \frac{[z_i(r) z_j(r)]'}{r} - \frac{\phi(r)}{r}$$

and,

$$\phi''(r) = \frac{[z_i(r) z_j(r)]''}{r} - \frac{2[\phi(r)]'}{r}$$

EAM force is defined by

$$\mathcal{F}_k = -\frac{d\mathcal{E}}{dx_k}$$

$$\mathcal{F}_k = \left[\frac{dE^e}{dx_k} + \frac{d\Phi}{dx_k}\right]$$

where the pair potential component is

$$\frac{dE^e}{dx_k} = \sum_j^{n_k} \left[\rho_k'(r_{kj})E_j'(\bar{\rho}_j) + \rho_j'(r_{kj})E_k'(\bar{\rho}_k)\right] \frac{\vec{r}_{kj}}{r_{kj}}$$

and, the embedded energy component is

$$\frac{d\Phi}{dx_k} = \sum_j^{n_k} \phi'(r_{kj})\frac{\vec{r}_{kj}}{r_{kj}}$$

Finally, the total force is

$$\mathcal{F}_k = \sum_j^{n_k} \left[\rho_k'(r_{jk})E_j'(\bar{\rho}_j) + \rho_j'(r_{jk})E_k'(\bar{\rho}_k) + \phi'(r_{jk})\right] \frac{\vec{r}_{jk}}{r_{jk}}$$

3 EAM Tangent

EAM tangent matrix is defined by

$$\begin{aligned}\mathcal{S}_{ij} &= -\frac{d\mathcal{F}_j}{dx_i} \\ &= \frac{d^2\mathcal{E}}{dx_i dx_j}\end{aligned}$$

$$\mathcal{S}_{ij} = \frac{d^2E^e}{dx_i dx_j} + \frac{1}{2}\frac{d^2\Phi}{dx_i dx_j}$$

The tangent matrix for the pair potential is given by
First case : $\underline{i = j}$

$$\frac{d^2\Phi}{dx_i^2} = -\sum_k^{n_i} \left\{\phi''(r_{ik})\frac{\vec{r}_{ik}}{r_{ik}}\frac{\vec{r}_{ik}}{r_{ik}} + \frac{\phi'(r_{ik})}{r_{ik}}\left(1 - \frac{\vec{r}_{ik}}{r_{ik}}\frac{\vec{r}_{ik}}{r_{ik}}\right)\right\}$$

Second case : $\underline{i \neq j}$

$$\frac{d^2\Phi}{dx_i dx_j} = \phi''(r_{ij})\frac{\vec{r}_{ij}}{r_{ij}}\frac{\vec{r}_{ij}}{r_{ij}} + \frac{\phi'(r_{ij})}{r_{ij}}\left(1 - \frac{\vec{r}_{ij}}{r_{ij}}\frac{\vec{r}_{ij}}{r_{ij}}\right)$$

The tangent matrix for the embedded energy is given by
First case : $\underline{i = j}$

$$\frac{d^2E^e}{dx_i^2} = -\sum_k^{n_i} \left\{\frac{E_{ik}}{r_{ik}} + (K_{ik} - \frac{E_{ik}}{r_{ik}})\frac{\vec{r}_{ik}}{r_{ik}}\frac{\vec{r}_{ik}}{r_{ik}} + T_{ik}\right\}$$

where we have posed

$$\begin{aligned}
F_{ik} &= \rho_i'(r_{ik})E_k'(\bar{\rho}_k) + \rho_k'(r_{ik})E_i'(\bar{\rho}_i) \\
K_{ik} &= \rho_i''(r_{ik})E_k'(\bar{\rho}_k) + \rho_k''(r_{ik})E_i'(\bar{\rho}_i)(\bar{\rho}_k) + [\rho_i'(r_{ik})]^2 E_k''(\bar{\rho}_k) \\
T_{ik} &= E_i''(\bar{\rho}_i)\rho_k'(r_{ik}) \left(\sum_l^{n(i)} \rho_l'(r_{il}) \frac{\vec{r}_{il}}{r_{il}} \right) \frac{\vec{r}_{ik}}{r_{ik}}
\end{aligned}$$

Second case : $\underline{i \neq j}$

$$\frac{d^2E^e}{dx_i dx_j} = \frac{E_{ij}'}{r_{ij}} + (K_{ij} - \frac{E_{ij}'}{r_{ij}})\frac{\vec{r}_{ij}}{r_{ij}}\frac{\vec{r}_{ij}}{r_{ij}} + T_{ij}$$

where we have posed

$$\begin{aligned}
F_{ij} &= \rho_i'(r_{ij})E_j'(\bar{\rho}_j) + \rho_j'(r_{ij})E_i'(\bar{\rho}_j) \\
K_{ij} &= \rho_i''(r_{ij})E_j'(\bar{\rho}_j) + \rho_j''(r_{ij})E_i'(\bar{\rho}_i) \\
T_{ij} &= (\rho_j'(r_{ij})E_i''(\bar{\rho}_i) - \rho_i'(r_{ij})E_j''(\bar{\rho}_j)) \left(\sum_k^{n(i)} \rho_k'(r_{ik}) \frac{\vec{r}_{ik}}{r_{ik}} \right) \frac{\vec{r}_{ij}}{r_{ij}} + \sum_k^{n(i),n(j)} \rho_i'(r_{ik})\rho_j'(r_{kj})E_k'' \frac{\vec{r}_{ik}}{r_{ik}}\frac{\vec{r}_{kj}}{r_{kj}}
\end{aligned}$$