

Additional documentation for the Gay-Berne ellipsoidal potential as implemented in LAMMPS

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The Gay-Berne anisotropic LJ interaction between pairs of dissimilar ellipsoidal particles is given by

$$U(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}) = \mathbf{U}_r(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}, \gamma) \cdot \eta_{12}(\mathbf{A}_1, \mathbf{A}_2, v) \cdot \chi_{12}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}, \mu)$$

where \mathbf{A}_1 and \mathbf{A}_2 are the transformation matrices from the simulation box frame to the body frame and \mathbf{r}_{12} is the center to center vector between the particles. U_r controls the shifted distance dependent interaction based on the distance of closest approach of the two particles (h_{12}) and the user-specified shift parameter gamma:

$$U_r = 4\epsilon(\varrho^{12} - \varrho^6)$$

$$\varrho = \frac{\sigma}{h_{12} + \gamma\sigma}$$

Let the shape matrices $\mathbf{S}_i = \text{diag}(\mathbf{a}_i, \mathbf{b}_i, \mathbf{c}_i)$ be given by the ellipsoid radii. The η orientation-dependent energy based on the user-specified exponent v is given by

$$\eta_{12} = \left[\frac{2s_1s_2}{\det(\mathbf{G}_{12})} \right]^{v/2},$$

$$s_i = [a_ib_i + c_ic_i][a_ib_i]^{1/2},$$

and

$$\mathbf{G}_{12} = \mathbf{A}_1^T \mathbf{S}_1^2 \mathbf{A}_1 + \mathbf{A}_2^T \mathbf{S}_2^2 \mathbf{A}_2 = \mathbf{G}_1 + \mathbf{G}_2.$$

Let the relative energy matrices $\mathbf{E}_i = \text{diag}(\epsilon_{ia}, \epsilon_{ib}, \epsilon_{ic})$ be given by the relative well depths (dimensionless energy scales inversely proportional to the well-depths of the respective orthogonal configurations of the interacting

molecules). The χ orientation-dependent energy based on the user-specified exponent μ is given by

$$\chi_{12} = [2\hat{\mathbf{r}}_{12}^T \mathbf{B}_{12}^{-1} \hat{\mathbf{r}}_{12}]^\mu,$$

$$\hat{\mathbf{r}}_{12} = \mathbf{r}_{12}/|\mathbf{r}_{12}|,$$

and

$$\mathbf{B}_{12} = \mathbf{A}_1^T \mathbf{E}_1^2 \mathbf{A}_1 + \mathbf{A}_2^T \mathbf{E}_2^2 \mathbf{A}_2 = \mathbf{B}_1 + \mathbf{B}_2.$$

Here, we use the distance of closest approach approximation given by the Perram reference, namely

$$h_{12} = r - \sigma_{12}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}),$$

$$r = |\mathbf{r}_{12}|,$$

and

$$\sigma_{12} = [\frac{1}{2}\hat{\mathbf{r}}_{12}^T \mathbf{G}_{12}^{-1} \hat{\mathbf{r}}_{12}]^{-1/2}$$

Forces and Torques: Because the analytic forces and torques have not been published for this potential, we list them here:

$$\mathbf{f} = -\eta_{12}(\mathbf{U}_r \cdot \frac{\partial \chi_{12}}{\partial \mathbf{r}} + \chi_{12} \cdot \frac{\partial \mathbf{U}_r}{\partial \mathbf{r}})$$

where the derivative of U_r is given by (see Allen reference)

$$\frac{\partial U_r}{\partial r} = \frac{\partial U_{SLJ}}{\partial r} \hat{\mathbf{r}}_{12} + r^{-2} \frac{\partial U_{SLJ}}{\partial \varphi} [\kappa - (\kappa^T \cdot \hat{\mathbf{r}}_{12}) \hat{\mathbf{r}}_{12}],$$

$$\frac{\partial U_{SLJ}}{\partial \varphi} = 24\epsilon(2\varrho^{13} - \varrho^7)\sigma_{12}^3/2\sigma,$$

$$\frac{\partial U_{SLJ}}{\partial r} = 24\epsilon(2\varrho^{13} - \varrho^7)/\sigma,$$

and

$$\kappa = \mathbf{G}_{12}^{-1} \cdot \mathbf{r}_{12}.$$

The derivate of the χ term is given by

$$\frac{\partial \chi_{12}}{\partial r} = -r^{-2} \cdot 4.0 \cdot [\iota - (\iota^{\mathbf{T}} \cdot \hat{\mathbf{r}}_{12}) \hat{\mathbf{r}}_{12}] \cdot \mu \cdot \chi_{12}^{(\mu-1)/\mu},$$

and

$$\iota = \mathbf{B}_{12}^{-1} \cdot \mathbf{r}_{12}.$$

The torque is given by:

$$\tau_{\mathbf{i}} = \mathbf{U}_{\mathbf{r}} \eta_{12} \frac{\partial \chi_{12}}{\partial \mathbf{q}_{\mathbf{i}}} + \chi_{12} (\mathbf{U}_{\mathbf{r}} \frac{\partial \eta_{12}}{\partial \mathbf{q}_{\mathbf{i}}} + \eta_{12} \frac{\partial \mathbf{U}_{\mathbf{r}}}{\partial \mathbf{q}_{\mathbf{i}}}),$$

$$\frac{\partial U_r}{\partial \mathbf{q}_{\mathbf{i}}} = \mathbf{A}_{\mathbf{i}} \cdot (-\kappa^{\mathbf{T}} \cdot \mathbf{G}_{\mathbf{i}} \times \mathbf{f}_{\mathbf{k}}),$$

$$\mathbf{f}_{\mathbf{k}} = -\mathbf{r}^{-2} \frac{\delta \mathbf{U}_{\text{SLJ}}}{\delta \varphi} \kappa,$$

and

$$\frac{\partial \chi_{12}}{\partial \mathbf{q}_{\mathbf{i}}} = 4.0 \cdot r^{-2} \cdot \mathbf{A}_{\mathbf{i}} (-\iota^{\mathbf{T}} \cdot \mathbf{B}_{\mathbf{i}} \times \iota).$$

For the derivative of the η term, we were unable to find a matrix expression due to the determinant. Let a_{mi} be the m th row of the rotation matrix A_i . Then,

$$\frac{\partial \eta_{12}}{\partial \mathbf{q}_{\mathbf{i}}} = \mathbf{A}_{\mathbf{i}} \cdot \sum_{\mathbf{m}} \mathbf{a}_{\mathbf{m}\mathbf{i}} \times \frac{\partial \eta_{12}}{\partial \mathbf{a}_{\mathbf{m}\mathbf{i}}} = \mathbf{A}_{\mathbf{i}} \cdot \sum_{\mathbf{m}} \mathbf{a}_{\mathbf{m}\mathbf{i}} \times \mathbf{d}_{\mathbf{m}\mathbf{i}},$$

where d_{mi} represents the m th row of a derivative matrix D_i ,

$$\mathbf{D}_{\mathbf{i}} = -\frac{1}{2} \cdot \left(\frac{2\mathbf{s}_1\mathbf{s}_2}{\det(\mathbf{G}_{12})} \right)^{v/2} \cdot \frac{v}{\det(\mathbf{G}_{12})} \cdot \mathbf{E},$$

where the matrix E gives the derivate with respect to the rotation matrix,

$$\mathbf{E} = [\mathbf{e}_{\mathbf{m}\mathbf{y}}] = \frac{\partial \eta_{12}}{\partial \mathbf{A}_{\mathbf{i}}},$$

and

$$e_{my} = \det(\mathbf{G}_{12}) \cdot \text{trace}[\mathbf{G}_{12}^{-1} \cdot (\hat{\mathbf{p}}_y \otimes \mathbf{a}_m + \mathbf{a}_m \otimes \hat{\mathbf{p}}_y) \cdot \mathbf{s}_{mm}^2].$$

Here, p_v is the unit vector for the axes in the lab frame ($p1 = [1, 0, 0]$, $p2 = [0, 1, 0]$, and $p3 = [0, 0, 1]$) and s_{mm} gives the m th radius of the ellipsoid i .