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

\[ U(A_1, A_2, r_{12}) = U_r(A_1, A_2, r_{12}, \gamma) \cdot \eta_{12}(A_1, A_2, \nu) \cdot \chi_{12}(A_1, A_2, r_{12}, \mu) \]

where \( A_1 \) and \( A_2 \) are the transformation matrices from the simulation box frame to the body frame and \( r_{12} \) 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 \( \gamma \):

\[ U_r = 4\epsilon(\varrho_{12}^\nu - \varrho^\nu) \]

\[ \varrho = \frac{\sigma}{h_{12} + \gamma\sigma} \]

Let the shape matrices \( S_i = \text{diag}(a_i, b_i, c_i) \) be given by the ellipsoid radii. The \( \eta \) orientation-dependent energy based on the user-specified exponent \( \nu \) is given by

\[ \eta_{12} = \left[ \frac{2s_1s_2}{\det(G_{12})} \right]^\nu/2, \]

\[ s_i = [a_1b_1 + c_1c_i][a_i]^{1/2}, \]

and

\[ G_{12} = A_1^T S_1^2 A_1 + A_2^T S_2^2 A_2 = G_1 + G_2. \]

Let the relative energy matrices \( E_i = \text{diag}(\epsilon_{ia}^{-1/\mu}, \epsilon_{ib}^{-1/\mu}, \epsilon_{ic}^{-1/\mu}) \) 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 $\chi$ orientation-dependent energy based on the user-specified exponent $\mu$ is given by

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

and

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

and

$$B_{12} = A_1^T E_1 A_1 + A_2^T E_2 A_2 = B_1 + B_2.$$

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

$$h_{12} = r - \sigma_{12}(A_1, A_2, r_{12}),$$

$$r = |r_{12}|,$$

and

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

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

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

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

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

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

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

and
\[ \kappa = G^{-1}_{12} \cdot r_{12}. \]

The derivative of the \( \chi \) term is given by
\[
\frac{\partial \chi_{12}}{\partial r} = -r^{-2} \cdot 4.0 \cdot \left[ \kappa - (\iota^T \cdot \hat{r}_{12}) \hat{r}_{12} \right] \cdot \mu \cdot \chi^{(\mu-1)/\mu}_{12},
\]
and
\[
\iota = B^{-1}_{12} \cdot r_{12}.
\]

The torque is given by:
\[
\tau_i = U_r \eta_{12} \frac{\partial \chi_{12}}{\partial q_i} + \chi_{12} (U_r \frac{\partial \eta_{12}}{\partial q_i} + \eta_{12} \frac{\partial U_r}{\partial q_i}),
\]
\[
\frac{\partial U_r}{\partial q_i} = A_i \cdot (-\kappa^T \cdot G_i \times f_k),
\]
\[
f_k = -r^{-2} \frac{\delta U_{SLJ}}{\delta \varphi} \kappa,
\]
and
\[
\frac{\partial \chi_{12}}{\partial q_i} = 4.0 \cdot r^{-2} \cdot A_i (-\iota^T \cdot B_i \times \iota) \cdot \mu \cdot \chi^{(\mu-1)/\mu}_{12}.
\]

For the derivative of the \( \eta \) term, we were unable to find a matrix expression due to the determinant. Let \( a_{mi} \) be the mth row of the rotation matrix \( A_i \). Then,
\[
\frac{\partial \eta_{12}}{\partial q_i} = A_i \cdot \sum_m a_{mi} \times \frac{\partial \eta_{12}}{\partial a_{mi}} = A_i \cdot \sum_m \, a_{mi} \times d_{mi},
\]
where \( d_{mi} \) represents the mth row of a derivative matrix \( D_i \),
\[
D_i = -\frac{1}{2} \cdot \left( \frac{2s1s2}{\det(G_{12})} \right)^{v/2} \cdot \frac{v}{\det(G_{12})} \cdot E,
\]
where the matrix \( E \) gives the derivative with respect to the rotation matrix,
\[
E = [e_{my}] = \frac{\partial \eta_{12}}{\partial A_i},
\]
\[ \text{3} \]
and

\[ e_{my} = \det(G_{12}) \cdot \text{trace}[G_{12}^{-1} \cdot (\hat{p}_y \otimes a_m + a_m \otimes \hat{p}_y) \cdot s_{mm}^2]. \]

Here, \( p_v \) is the unit vector for the axes in the lab frame \( (p_1 = [1, 0, 0], p_2 = [0, 1, 0], \text{and} p_3 = [0, 0, 1]) \) and \( s_{mm} \) gives the \( m \)th radius of the ellipsoid \( i \).