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

$$U(\mathbf{A_1}, \mathbf{A_2}, \mathbf{r_{12}}) = \mathbf{U_r}(\mathbf{A_1}, \mathbf{A_2}, \mathbf{r_{12}}, \gamma) \cdot \eta_{\mathbf{12}}(\mathbf{A_1}, \mathbf{A_2}, \upsilon) \cdot \chi_{\mathbf{12}}(\mathbf{A_1}, \mathbf{A_2}, \mathbf{r_{12}}, \mu)$$

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 $\mathbf{S_i} = \mathrm{diag}(\mathbf{a_i}, \mathbf{b_i}, \mathbf{c_i})$ be given by the ellipsoid radii. The η orientation-dependent energy based on the user-specified exponent υ is given by

$$\eta_{12} = [\frac{2s_1 s_2}{\det(\mathbf{G_{12}})}]^{\upsilon/2},$$

$$s_i = [a_i b_i + c_i c_i][a_i b_i]^{1/2},$$

and

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

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

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

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

and

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

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

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

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

and

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

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

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

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

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

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

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

and

$$\kappa = \mathbf{G_{12}^{-1}} \cdot \mathbf{r_{12}}.$$

The derivate of the χ term is given by

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

and

$$\iota = \mathbf{B_{12}^{-1}} \cdot \mathbf{r_{12}}.$$

The torque is given by:

$$\tau_{\mathbf{i}} = \mathbf{U_r}\eta_{\mathbf{12}}\frac{\partial \chi_{\mathbf{12}}}{\partial \mathbf{q_i}} + \chi_{\mathbf{12}}(\mathbf{U_r}\frac{\partial \eta_{\mathbf{12}}}{\partial \mathbf{q_i}} + \eta_{\mathbf{12}}\frac{\partial \mathbf{U_r}}{\partial \mathbf{q_i}}),$$

$$\frac{\partial U_r}{\partial \mathbf{q_i}} = \mathbf{A_i} \cdot (-\kappa^{\mathbf{T}} \cdot \mathbf{G_i} \times \mathbf{f_k}),$$

$$\mathbf{f_k} = -\mathbf{r}^{-\mathbf{2}}\frac{\delta \mathbf{U_{SLJ}}}{\delta \varphi}\kappa,$$

and

$$\frac{\partial \chi_{12}}{\partial \mathbf{q_i}} = 4.0 \cdot r^{-2} \cdot \mathbf{A_i}(-\iota^{\mathbf{T}} \cdot \mathbf{B_i} \times \iota).$$

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

$$\frac{\partial \eta_{12}}{\partial \mathbf{q_i}} = \mathbf{A_i} \cdot \sum_{\mathbf{m}} \mathbf{a_{mi}} \times \frac{\partial \eta_{\mathbf{12}}}{\partial \mathbf{a_{mi}}} = \mathbf{A_i} \cdot \sum_{\mathbf{m}} \mathbf{a_{mi}} \times \mathbf{d_{mi}},$$

where $d_m i$ represents the mth row of a derivative matrix D_i,

$$\mathbf{D_i} = -\frac{\mathbf{1}}{\mathbf{2}} \cdot (\frac{\mathbf{2s1s2}}{\det(\mathbf{G_{12}})})^{\upsilon/\mathbf{2}} \cdot \frac{\upsilon}{\det(\mathbf{G_{12}})} \cdot \mathbf{E},$$

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

$$\mathbf{E} = [\mathbf{e_{my}}] = \frac{\partial \eta_{\mathbf{12}}}{\partial \mathbf{A_i}},$$

and

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

Here, p_v is the unit vector for the axes in the lab frame ($p1 = [1, 0, 0], p2 = [0, 1, 0], andp3 = [0, 0, 1]$) and s_{mm} gives the mth radius of the ellipsoid i.