Additional documentation for the RE-squared ellipsoidal potential as implemented in LAMMPS

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Let the shape matrices $\mathbf{S_i} = \mathrm{diag}(\mathbf{a_i}, \mathbf{b_i}, \mathbf{c_i})$ be given by the ellipsoid radii. Let the relative energy matrices $\mathbf{E_i} = \mathrm{diag}(\epsilon_{\mathbf{ia}}, \epsilon_{\mathbf{ib}}, \epsilon_{\mathbf{ic}})$ 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). Let $\mathbf{A_1}$ and $\mathbf{A_2}$ be the transformation matrices from the simulation box frame to the body frame and $\mathbf{r}$ be the center to center vector between the particles. Let A_{12} be the Hamaker constant for the interaction given in LJ units by $A_{12} = 4\pi^2\epsilon_{\mathrm{LJ}}(\rho\sigma^3)^2$.

The RE-squared anisotropic interaction between pairs of ellipsoidal particles is given by

$$U = U_A + U_R,$$

$$U_\alpha = \frac{A_{12}}{m_\alpha}(\frac{\sigma}{h})^{n_\alpha}(1 + o_\alpha\eta\chi\frac{\sigma}{h}) \times \prod_i \frac{a_i b_i c_i}{(a_i + h/p_\alpha)(b_i + h/p_\alpha)(c_i + h/p_\alpha)},$$

$$m_A = -36, n_A = 0, o_A = 3, p_A = 2,$$

$$m_R = 2025, n_R = 6, o_R = 45/56, p_R = 60^{1/3},$$

$$\chi = 2\hat{\mathbf{r}}^T\mathbf{B^{-1}}\hat{\mathbf{r}},$$

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

$$\mathbf{B} = \mathbf{A_1^T E_1 A_1} + \mathbf{A_2^T E_2 A_2}$$

$$\eta = \frac{\det[\mathbf{S_1}]/\sigma_\mathbf{1}^\mathbf{2} + \mathbf{det}[\mathbf{S_2}]/\sigma_\mathbf{2}^\mathbf{2}}{[\det[\mathbf{H}]/(\sigma_\mathbf{1}+\sigma_\mathbf{2})]^{\mathbf{1/2}}},$$

$$\sigma_i = (\hat{\mathbf{r}}^T \mathbf{A_i^T S_i^{-2} A_i} \hat{\mathbf{r}})^{-\mathbf{1/2}},$$

$$\mathbf{H} = \frac{\mathbf{1}}{\sigma_\mathbf{1}} \mathbf{A_1^T S_1^2 A_1} + \frac{\mathbf{1}}{\sigma_\mathbf{2}} \mathbf{A_2^T S_2^2 A_2}$$

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

$$h = |r| - \sigma_{12},$$

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

and

$$\mathbf{G} = \mathbf{A_1^T S_1^2 A_1} + \mathbf{A_2^T S_2^2 A_2}$$

The RE-squared anisotropic interaction between a ellipsoidal particle and a Lennard-Jones sphere is defined as the $\lim_{a_2 -> 0} U$ under the constraints that $a_2 = b_2 = c_2$ and $\frac{4}{3}\pi a_2^3 \rho = 1$:

$$U_{\text{elj}} = U_{A_{\text{elj}}} + U_{R_{\text{elj}}},$$

$$U_{\alpha_{\text{elj}}} = (\frac{3\sigma^3 c_\alpha^3}{4\pi h_{\text{elj}}^3}) \frac{A_{12_{\text{elj}}}}{m_\alpha} (\frac{\sigma}{h_{\text{elj}}})^{n_\alpha} (1 + o_\alpha \chi_{\text{elj}} \frac{\sigma}{h_{\text{elj}}}) \times \frac{a_1 b_1 c_1}{(a_1 + h_{\text{elj}}/p_\alpha)(b_1 + h_{\text{elj}}/p_\alpha)(c_1 + h_{\text{elj}}/p_\alpha)},$$

$$A_{12_{\text{elj}}} = 4\pi^2 \epsilon_{\text{LJ}} (\rho\sigma^3),$$

with h_{elj} and χ_{elj} calculated as above by replacing B with B_{elj} and G with G_{elj}:

$$\mathbf{B}_{\text{elj}} = \mathbf{A_1^T E_1 A_1} + \mathbf{I},$$

$$\mathbf{G}_{\mathrm{elj}} = \mathbf{A_1^T S_1^2 A_1}.$$

The interaction between two LJ spheres is calculated as:

$$U_{\mathrm{lj}} = 4\epsilon \left[\left(\frac{\sigma}{|\mathbf{r}|} \right)^{12} - \left(\frac{\sigma}{|\mathbf{r}|} \right)^{6} \right]$$

The analytic derivatives are used for all force and torque calculation.