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

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

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

$$U = U_A + U_R,$$

$$U_A = \frac{A_{12} \sigma}{m_A} \left( \frac{\sigma}{h} \right)^{m_A} (1 + o_A \chi \frac{\sigma}{h}) \times \prod_i \frac{a_i b_i c_i}{(a_i + h/p \alpha)(b_i + h/p \alpha)(c_i + h/p \alpha)},$$

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

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

$$\chi = 2\tilde{r}^T \text{B}^{-1} \tilde{r},$$

$$\tilde{r} = r/|r|,$$

$$\text{B} = A_1^T E_1 A_1 + A_2^T E_2 A_2$$
\[
\eta = \frac{\det[S_1]/\sigma_1^2 + \det[S_2]/\sigma_2^2}{[\det[H]/(\sigma_1 + \sigma_2)]^{1/2}},
\]
\[
\sigma_i = (\hat{r}_i^T A_i^T S_i^{-2} A_i \hat{r})^{-1/2},
\]
\[
H = \frac{1}{\sigma_1} A_1^T S_1^2 A_1 + \frac{1}{\sigma_2} A_2^T S_2^2 A_2
\]

H \quad \text{Here, we use the distance of closest approach approximation given by the Perram reference, namely}

\[
h = |r| - \sigma_{12},
\]
\[
\sigma_{12} = [\frac{1}{2} \hat{r}_G^T G^{-1} \hat{r}]^{-1/2},
\]

and

\[
G = A_1^T S_1^2 A_1 + A_2^T S_2^2 A_2
\]

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

\[
U_{elj} = U_{A_{elj}} + U_{R_{elj}},
\]

\[
U_{A_{elj}} = \left( \frac{3 \sigma_3^3 \rho^3}{4 \pi h_{elj}^3} \right) \frac{A_{12_{elj}}}{m_\alpha} \frac{\sigma}{h_{elj}} (1+o_\alpha \chi_{elj}) \frac{\sigma}{\sigma_0} \times \frac{a_1 b_1 c_1}{(a_1 + h_{elj}/p_\alpha)(b_1 + h_{elj}/p_\alpha)(c_1 + h_{elj}/p_\alpha)},
\]

\[
A_{12_{elj}} = 4 \pi^2 \epsilon_{elj}(\rho \sigma^3),
\]

with \( h_{elj} \) and \( \chi_{elj} \) calculated as above by replacing \( B \) with \( B_{elj} \) and \( G \) with \( G_{elj} \):

\[
B_{elj} = A_1^T E_1 A_1 + I,
\]
\[ G_{elj} = A_1^T S_1^2 A_1. \]

The interaction between two LJ spheres is calculated as:

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

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