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 $\frac{4}{3}\pi a_2^3 \rho = 1$:

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

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

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

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

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

The distance of closest approach approximation becomes inaccurate for disparate sizes, even for spherical particles. For spheres, with radii a_1 and a_2 the contact distance using this approximation is $\sqrt{2(a_1^2 + a_2^2)}$ rather than $a_1 + a_2$. This can lead to large errors when calculating distances between large ellipsoids and small solvent particles. Therefore, we have corrected the distance of closest approach approximation for interactions between ellipsoids and spherical LJ particles to account for this error. The distance of closest approach in this case, h_{elj}, is calculated as described above but replacing $\mathbf{G}$ with $\mathbf{G}_{\mathrm{elj}}$:

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

where $\hat{\mathbf{C}} = \mathrm{diag}[\frac{(a_i+\sigma/2)^2}{2a_i^2}, \frac{(b_i+\sigma/2)^2}{2b_i^2}, \frac{(c_i+\sigma/2)^2}{2c_i^2}]$. Note that this assumes a spherical LJ particle with radius $\sigma/2$.

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.