Linear overlap to volume overlap

October 22, 2021

Chapter 1

Intro

The aim of this document is to explain the formulae behind function getOverlapVolume. This function is part of the interaction and returns the effect volume overlap (at the moment assuming spheres). In the next section is the maths behind this formulae and also in the directory is the mathematica notebook to do the calculation (OverlapVolume.nb).

Chapter 2

The Math

Given overlap δ and particle radii r_1, r_2, we want to the overlap volume V.

First we compute the thickness of the spherical caps, $t_1 = r_1 - a$ and $t_2 = r_2 - b$, in the diagram below.
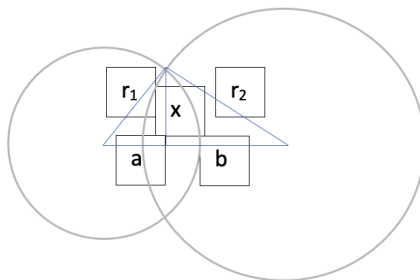
We know

$$x^2 = r_1^2 - a^2, \quad x^2 = r_2^2 - b^2, \quad a + b = r_1 + r_2 - \delta$$

Thus

$$r_1^2 - a^2 = r_2^2 - (r_1 + r_2 - \delta - a)^2$$

Mathematica yields with the following commands:

```
Simplify[r1 - a /. Solve[r1^2 - a^2 == r2^2 - (r1 + r2 - d - a)^2, a]]
```

$$t_1 = r_1 - a = \frac{r_2 - \delta/2}{r_1 + r_2 - \delta}\delta \tag{2.1}$$

$$t_2 = r_2 - b = \frac{r_1 - \delta/2}{r_1 + r_2 - \delta}\delta \tag{2.2}$$

Thus, the volume of the two spherical caps is

$$V = \pi \left\{ \int_0^{t_1} r_1^2 - r^2 dr + \int_0^{t_2} r_2^2 - r^2 dr \right\}$$

$$V = \pi \left\{ r_1^2 t_1 - t_1^3/3 + r_2^2 t_2 - t_2^3/3 \right\} \tag{2.3}$$

It seems, this cannot be simplified further. The full expression in terms of r_1, r_2, δ is

$$V = \pi \left\{ \frac{-\delta^3(\delta - 2r_2)^3 - 12r_2^2(-\delta + r_1 + r_2)^2 \left(\delta^2 - 2\delta(r_1 + r_2) + 2r_2(r_1 + r_2)\right) + \left(\delta^2 - 2\delta(r_1 + r_2) + 2r_2(r_1 + r_2)\right)^3 + 12\delta r_1^2(\delta - 2r_2)(-\delta + r_1 + r_2)^2}{24(\delta - r_1 - r_2)^3} \right\}$$