Generalization of the Rotne-Prager-Yamakawa mobility and shear disturbance tensors -other supplementary materials

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1. Calculation of integrals for overlapping particles

The configuration of the two spheres i and j and the notation is presented on figure 1. The z axis is chosen in the direction of the vector $\mathbf{R}_{ij}$ connecting the centres of the spheres. The variable $\mathbf{r}_i$ is a position vector from the centre of the sphere i and thus $\mathbf{r}'$ - a position vector from the centre of the sphere j. To demonstrate the method it is enough to calculate explicitely one of the integrals appearing in (3.6)-(3.7) and (3.21)-(3.22).We take the first one,

$$\mathbf{u}^t\left(\mathbf{R}_{ij}\right) = \frac{1}{4\pi a^2}\int_{S_i} \mathbf{v}_0^t\left(\mathbf{r}'\right)\mathrm{d}\sigma_i. \tag{1.1}$$

The integration is done over the surface of sphere i, thus $\mathbf{r}_i$ is expressed in spherical coordinates (r, θ, ϕ) associated with sphere i which leads to

$$\boldsymbol{\mu}_{ij}^{tt} = \frac{1}{32\pi^2\eta}\int_0^{\theta_0}\mathrm{d}\theta\sin\theta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{r'}\left[\left(1+\frac{a^2}{3r'^2}\right)\mathbf{1}+\left(1-\frac{a^2}{r'^2}\right)\hat{\mathbf{r}}'\hat{\mathbf{r}}'\right]+\frac{1}{2\zeta^{tt}}\mathbf{1}\left(1-\frac{R_{ij}}{2a}\right), \tag{1.2}$$

where θ_0 is the meridional angle at which the two spheres intersect (see figure 1), defined by

$$\cos\theta_0 = -\frac{R_{ij}}{2a}, \tag{1.3}$$

and the vector $\mathbf{r}' = \mathbf{R}_{ij} + \mathbf{r}_i$ in the cartesian basis has the form

$$\mathbf{r}' = a\sin\theta\cos\phi\hat{\mathbf{e}}_x + a\sin\theta\sin\phi\hat{\mathbf{e}}_y + \left(R_{ij}+a\cos\theta\right)\hat{\mathbf{e}}_z, \qquad r'^2 = R_{ij}^2 + 2R_{ij}a\cos\theta + a^2. \tag{1.4}$$

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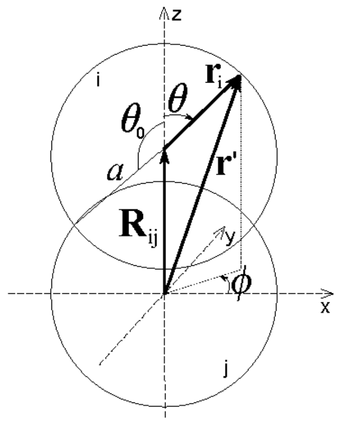

Figure 1. The axes positions and notation for calculation of the expressions for overlapping spheres.

The last term in (1.2) results from integration of the $r \leq a$ expression in (3.2) from θ_0 to π. All the azimuthal integrals in (1.2) are easily done to give

$$\boldsymbol{\mu}_{ij}^{tt} = \frac{1}{\zeta^{tt}}\mathbf{1}\left[\frac{1}{2}\left(1-\frac{R_{ij}}{2a}\right)+\frac{3}{8}\int_0^{\theta_0}\mathrm{d}\theta\sin\theta\left(\frac{a}{r'}+\frac{a^3}{3r'^3}\right)+\frac{3}{16}\int_0^{\theta_0}\mathrm{d}\theta\sin^3\theta\left(\frac{a^3}{r'^3}-\frac{a^5}{r'^5}\right)\right]$$
$$+\frac{3}{16\zeta^{tt}}\hat{\mathbf{R}}_{ij}\hat{\mathbf{R}}_{ij}\int_0^{\theta_0}\mathrm{d}\theta\sin\theta\left(\frac{a^3}{r'^3}-\frac{a^5}{r'^5}\right)\left[2\left(\frac{R_{ij}}{a}+\cos\theta\right)^2-\sin^2\theta\right], \tag{1.5}$$

and for the choice of coordinate axes as in figure 1 we have

$$\hat{\mathbf{R}}_{ij}\hat{\mathbf{R}}_{ij} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{1.6}$$

The calculation of $\boldsymbol{\mu}_{ij}^{tt}$ is now straightforward. Since

$$\int_0^{\theta_0}\mathrm{d}\theta\frac{a\sin\theta}{\left(R_{ij}^2+2R_{ij}a\cos\theta+a^2\right)^{1/2}} = 1, \tag{1.7}$$

$$\int_0^{\theta_0}\mathrm{d}\theta\frac{a^3\sin\theta}{\left(R_{ij}^2+2R_{ij}a\cos\theta+a^2\right)^{3/2}} = \frac{a}{R_{ij}+a}, \tag{1.8}$$

$$\int_0^{\theta_0}\mathrm{d}\theta\frac{a^3\sin^3\theta}{\left(R_{ij}^2+2R_{ij}a\cos\theta+a^2\right)^{3/2}} = \frac{8a-3R_{ij}}{12a}, \tag{1.9}$$

$$\int_0^{\theta_0}\mathrm{d}\theta\frac{a^5\sin^3\theta}{\left(R_{ij}^2+2R_{ij}a\cos\theta+a^2\right)^{5/2}} = \frac{-R_{ij}^2-R_{ij}a+8a^2}{12a\left(R_{ij}+a\right)}, \tag{1.10}$$

$$\int_0^{\theta_0}\mathrm{d}\theta\frac{a\sin\theta\left(R_{ij}+a\cos\theta\right)^2}{\left(R_{ij}^2+2R_{ij}a\cos\theta+a^2\right)^{3/2}} = \frac{3R_{ij}+4a}{12a}, \tag{1.11}$$

$$\int_0^{\theta_0}\mathrm{d}\theta\frac{a^3\sin\theta\left(R_{ij}+a\cos\theta\right)^2}{\left(R_{ij}^2+2R_{ij}a\cos\theta+a^2\right)^{5/2}} = \frac{R_{ij}^2+R_{ij}a+4a^2}{12a\left(R_{ij}+a\right)}, \tag{1.12}$$

the tt component of the mobility matrix takes the form

$$\boldsymbol{\mu}_{ij}^{tt} = \frac{1}{\zeta^{tt}} \left[\left(1 - \frac{9R_{ij}}{32a} \right) \mathbf{1} + \frac{3R_{ij}}{32a} \hat{\mathbf{R}}_{ij} \hat{\mathbf{R}}_{ij} \right], \tag{1.13}$$

as in (3.11).