Supplementary Materials:

Interaction Potentials from Arbitrary Multi-Particle Trajectory Data

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Generation of the Mobility Tensor

The terms of the mobility tensor, $\mathbf{D}$, are generated using the equations provided by Schmitz and Felderhof[1]. This approach generates a solution for $\mathbf{D}$ in the form of a series expansion, which has been solved for up to 12th order terms. The expression used for the self-interaction terms in the mobility tensor is given by

$$\mathbf{D}_{ii} = k_B T \left(4\pi\eta A_0^S\right)^{-1} \mathbf{I}\,, \tag{1}$$

where η is the viscosity of the fluid and A_0^S is a scattering coefficient. The two-particle interaction terms are generated using the expression

$$D_{ij,\alpha\beta}\left(\mathbf{R}_{ij}\right) = k_B T\left(\alpha\left(R_{ij}\right)\hat{R}_{ij,\alpha}\hat{R}_{ij,\beta} + \beta\left(R_{ij}\right)\left(\delta_{\alpha\beta} - \hat{R}_{ij,\alpha}\hat{R}_{ij,\beta}\right)\right), \tag{2}$$

where $\mathbf{r}_{ij}$ is the distance vector between a pair of particles, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and $\hat{R}_{ij,\alpha}$ is a normalized directional component of $\mathbf{r}_{ij}$ such that $\hat{R}_{ij,\alpha} = r_{ij,\alpha}/r_{ij}$. Values for the parameters α and β are found using

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\begin{aligned}
4\pi\eta\alpha\left(\mathbf{r}_{ij}\right) &= \frac{1}{2}r_{ij}^{-1} - \frac{1}{15}S_i r_{ij}^{-3} + A_{1,i}^S A_{1,j}^S r_{ij}^{-7} \\
&+ \left[A_{1,1}^S \left(-6B_{1,j}^S + \frac{18}{5}A_{2,j}^S + \frac{3}{5}\hat{B}_{2,j}^P \right) - \frac{2}{5}S_1 A_{1,i}^S A_{1,j}^S \right] r_{ij}^{-9} \\
&+ \left\{ A_{1,i}^S \left(-\frac{48}{5}B_{2,j}^S + \frac{40}{7}A_{3,j}^S + \frac{12}{7}B_{3,j}^P \right) - B_{1,i}^S \left(-5B_{1,j}^S + \frac{68}{5}A_{2,j}^S + \frac{3}{5}\hat{B}_{2,j}^P \right) \right. \\
&+ \mathrm{A}_{2,i}^S \left(\frac{21}{5}A_{2,j}^S + \frac{6}{5}B_{2,j}^P \right) - \frac{4}{5}S_i \left[A_{1,i}^S \left(-B_{1,\mathrm{j}}^S + \frac{3}{2}A_{2,j}^S \right) \right. \\
&+ \left. \left. \left(-\frac{3}{2}B_{1,i}^S + \frac{9}{10}A_{2,i}^S + \frac{3}{20}\hat{B}_{2,i}^P \right) A_{1,j}^S \right] + \frac{1}{450}S_i S_j A_{1,i}^S A_{i,j}^S \right\} r_{ij}^{-11} + [i \leftrightarrow j] + O\left(R_{ij}^{-13}\right)
\end{aligned}
\tag{3}
$$

$$
\begin{aligned}
4\pi\eta\beta(\mathbf{r}_{ij}) &= \frac{1}{4}r_{ij}^{-1} + \frac{1}{30}S_i r_{ij}^{-3} - \left\{ B_{1,i}^S \left(-\frac{1}{6}B_{1,j}^S + \frac{4}{15}A_{2,j}^S + \frac{2}{3}A_{2,j}^T + \frac{1}{10}\hat{B}_{2,j}^P \right) \right. \\
&+ A_{2,i}^S \left(\frac{61}{480}A_{2,j}^S + \frac{5}{12}A_{2,j}^T + \frac{3}{40}\hat{B}_{2,j}^P \right) - \frac{2}{3}A_{2,\mathrm{i}}^T A_{2,j}^T - \frac{1}{15}\mathrm{S}_i \\
&\mathrm{x}\left(-\mathrm{B}_{1,i}^S + \frac{4}{5}\mathrm{A}_{2,i}^S + 2\,\mathrm{A}_{2,i}^T + \frac{3}{10}\hat{\mathrm{B}}_{2,i}^P \right) \mathrm{A}_{1,j}^S \\
&+ \left. \frac{1}{150}\mathrm{S}_i\mathrm{S}_j\mathrm{A}_{1,i}^S\mathrm{A}_{1,\mathrm{j}}^S \right\} r_{ij}^{-11} + [i \leftrightarrow j] + O\left(R_{ij}^{-13}\right)
\end{aligned}
\tag{4}
$$

where the various $A_{m,i}^{\alpha}$ and $B_{m,i}^{\alpha}$ terms are scattering coefficients and S_i is given by

$$
\mathrm{S}_i = 3\frac{\mathrm{A}_{2,j}^P}{\mathrm{A}_{0,\mathrm{i}}^S}\,. \tag{5}
$$

The notation $[\mathrm{i} \leftrightarrow j]$ indicates that the equation should be repeated once with all *i* and *j* indices swapped[2].

REFERENCES

1 R. Schmitz and B. U. Felderhof, Physica A **116**, 163 (1982).
2 P. Reuland, B. U. Felderhof, and R. B. Jones, Physica A **93**, 465 (1978).