A Fast Multipole Method for the Rotne-Prager-Yamakawa tensor with different particle size

Edmond Chow Rohit Narurkar Vipul Harsh

May 30, 2014

FMM for RPY for Polydisperse Particle system

The Rpy tensor D(x,y) is defined as follows.

$$D(x,y) = \begin{cases} \frac{k_\beta T}{8\pi\eta}[(\frac{1}{r}\mathbf{I} + \frac{r\otimes r}{r^3}) + \frac{2a^2}{3r^3}(1 - 3\frac{r\otimes r}{r^2})] & r \geq a_x + a_y \\ \frac{k_\beta T}{6\pi\eta a}[(1 - \frac{9r}{32a})\mathbf{I} + \frac{3}{32a}\frac{r\otimes r}{r}] & r < a_x + a_y \end{cases}$$

In this report, we consider the calculation of the following sums.

$$u_i^m = \sum_{i=1}^{n}\sum_{j=1}^{3} D_{ij}(x^m, x^n)v_j^n$$

Where, x = $(x_1,\, x_2,\, x_3)$, y = $(y_1,\, y_2,\, y_3)$ are the position vectors of particle centers, a = $\frac{a_x^2+a_y^2}{2}$ and a_x and a_y are the radii of particles x and y respectively.

The classical FMM for coulombic interactions is as follows.

$$P^m(\text{q,p,d}) = \sum_{n=1,n\neq m}^{N} \frac{q^n}{r_{mn}} + \sum_{n=1,n\neq m}^{N} \frac{(d^n.r_{mn})p^n}{r_{mn}^3}$$

$$F_m^i(\text{q,p,d}) = \frac{\delta P^m(q,p,d)}{\delta x_i^m}$$

To make things simple, we assume that this sum is computed seperately as two sums, one for neighbouring particles and one for far away particles.

Revisiting our original goal,

$$u_i^m = \sum_{i=1}^{n}\sum_{j=1}^{3} D_{ij}(x^m, x^n)v_j^n \tag{1}$$

We split this sum in two, one for neighbouring particles and one for far particles.

$$u_i^m = u_{i,loc}^m + u_{i,far}^m$$

The ijth entry of D(x,y) can be rewritten as

$$\begin{aligned} D_{ij}(x,y) &= C_1\left(\frac{\mathbf{I}_{ij}}{|x-y|} + \frac{(x_i-y_i)(x_j-y_j)}{|x-y|^3}\right) + \frac{C_2(a_x^2+a_y^2)}{2}\left(\frac{\mathbf{I}_{ij}}{|x-y|^3} - \frac{(x_i-y_i)(x_j-y_j)}{|x-y|^5}\right) \\ &= C_1\left(\frac{\mathbf{I}_{ij}}{|x-y|} - (x_j-y_j)\frac{\delta}{\delta x_i}\frac{(x_i-y_i)}{|x-y|}\right) + \frac{C_2(a_x^2+a_y^2)}{2}\frac{\delta}{\delta x_i}\frac{(x_i-y_i)}{|x-y|^3} \end{aligned} \tag{2}$$

Where, $C_1 = \frac{k_\beta T}{8\pi\eta}$ and $C_2 = \frac{k_\beta T}{6\pi\eta}$ are constants.

Substituting this in **1**, we obtain

$$
\begin{aligned}
u_i^m &= \sum_{n \notin nborlist(m)} \sum_{j=1}^{3} D_{ij}(x^m, x^n) v_j^n \\
&= \sum_{n \notin nborlist(m)} \sum_{j=1}^{3} \left[C_1 \left(\frac{I_{ij}}{r_{mn}} - (x_j^m - x_j^n) \frac{\delta}{\delta x_i^m} \frac{1}{r_{mn}} \right) + C_2 \frac{(a_m^2 + a_n^2)}{2} \frac{\delta}{\delta x_i^m} \frac{x_j^m - x_j^n}{r_{mn}^3} \right] v_j^n \\
&= \sum_{n \notin nborlist(m)} C_1 \left(\frac{V_i^n}{r_{mn}} - \sum_{j=1}^{3} x_j^m \frac{\delta}{\delta x_j^m} \frac{v_j^n}{r_{mn}} + \frac{\delta}{\delta x_j^m} \frac{x^n . v^n}{r_{mn}} \right) + C_2 \frac{\delta}{\delta x_j^m} \frac{(\frac{a_n^2}{2} v^n) . r_{mn}}{r_{mn}} + \frac{a_m^2}{2} C_2 \frac{\delta}{\delta x_j^m} \frac{v^n . r_{mn}}{r_{mn}} \\
&= C_1 \sum_{n \notin nborlist(m)} \frac{V_i^n}{r_{mn}} - C_1 \sum_{j=1}^{3} x_j^m \frac{\delta}{\delta x_i^m} \sum_{n \notin nborlist(m)} \frac{v_j^n}{r_{mn}} + \frac{\delta}{\delta x_i^m} \left(\sum_{n \notin nborlist(m)} \frac{C_1 (x^n . v^n)}{r_{mn}} + \sum_{n \notin nborlist(m)} \frac{C_2 (\frac{a_n^2}{2} v^n . r_{mn})}{r_{mn}^3} \right) \\
&+ \frac{a_m^2}{2} \frac{\delta}{\delta x_i^m} \sum_{n \notin nborlist(m)} \frac{C_2 (v^n . r_{mn})}{r_{mn}^3}
\end{aligned}
\tag{3}
$$

This leads to the expression,

$$
u_{i,far}^m = C_1 P_{far}^m (v_i, 0, 0) - C_1 \sum_{j=1}^{3} x_j^m F_{i,far}^m (v_j, 0, 0) + F_{i,far}^m (C_1 (x.v), C_2, \frac{a_n^2}{2} v) + \frac{a_m^2}{2} F_{i,far}^m (0, C_2, v) \tag{4}
$$

In the fourth call, we let $(C_1 x^1 . v^1, C_1 x^2 . v^2, ..., C_1 x^n . v^n)$ be the charge strengths, $(C_2, C_2, ..., C_2)$ be the dipole strengths and $(\frac{a_1^2}{2} v^1, \frac{a_2^2}{2} v^2, ..., \frac{a_n^2}{2} v^n)$ be the dipole orientation vectors.

In the fifth call, we let (0, 0,...,0) be the charge strengths, $(C_2, C_2, ..., C_2)$ be the dipole strengths and $(v^1, v^2, ..., v^n)$ be the dipole orientation vectors.

In short, to compute $u_{i,far}^m$, we need to call the harmonic FMM five times, using the source locations $\{x_n\}$. Note that, the original goal was to compute u^m and not $u_{i,far}^m$. We still need to add the forces due to neighbouring particles. For this purpose we introduce the next step ***Post Correction***.

Post Correction

We call the harmonic library five times as stated in equation **4**. Note that this evaluates forces due to closer particles the same way as far away particles. For post correction, we first identify which particles are close. A naive way to do this is by simply looping over all pairs of particles. The complexity of this approach is $O(n^2)$ and is not scalable for a large number of particles. There are better ways to do this.