Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **13**, No. 2, pp. 296-310

DOI: 10.4208/aamm.OA-2019-0322
April 2021

# A Kernel-Independent Treecode for General Rotne-Prager-Yamakawa Tensor

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Received 4 November 2019; Accepted (in revised version) 3 March 2020

**Abstract.** A particle-cluster treecode based on barycentric Lagrange interpolation is presented for fast summation of hydrodynamic interactions through general Rotne-Prager-Yamakawa tensor in 3D. The interpolation nodes are taken to be Chebyshev points of the 2nd kind in each cluster. The barycentric Lagrange interpolation is scale-invariant that promotes the treecode's efficiency. Numerical results show that the treecode CPU time scales like $\mathcal{O}(N\log N)$, where $N$ is the number of beads in the system. The kernel-independent treecode is a relatively simple algorithm with low memory consumption, and this enables a straightforward OpenMP parallelization.

**AMS subject classifications**: 65D99, 76D07

**Key words**: General Rotne-Prager-Yamakawa tensor, fast summation, treecode, barycentric Lagrange interpolation.

## 1 Introduction

The Brownian Dynamics (BD) is a coarse-grained model used to account for long-range hydrodynamic interactions (HI) of small spherical particles suspended in a viscous flow at low Reynolds number. The technique is commonly used to study properties of rigid and flexible macromolecules using bead models [2,6,9,26]. Particle beads moving in a viscous fluid induce a local flow field that affects other beads. The long-range, many-body interactions, mediated by the solvent are commonly called HI. HIs are critical to describe large scale collective motions. The Ermak-McCammon algorithm is one of the popular algorithms for Brownian dynamics simulation with hydrodynamic interactions [7, 12], where the particles are assumed to be spherical beads, and hydrodynamic interactions between particles are described by a diffusion tensor. The Rotne-Prager-Yamakawa (RPY) approximation is one of the most commonly used tensors of including HIs in modeling

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of colloidal suspensions and polymer solutions [23, 30]. This widely used approach has been recently generalized by [27, 28] for the RPY translational and rotational degrees of freedom, as well as for the shear disturbance tensor $\boldsymbol{C}$ which gives the response of the particles to an external shear flow. The general Rotne-Prager-Yamakawa (GRPY) mobility has the form

$$\boldsymbol{\mu}=\begin{pmatrix} \boldsymbol{\mu}^{tt} & \boldsymbol{\mu}^{tr} \\ \boldsymbol{\mu}^{rt} & \boldsymbol{\mu}^{rr} \end{pmatrix}=\begin{pmatrix} \mu_{11}^{tt} & \cdots & \mu_{1N}^{tt} & \mu_{11}^{tr} & \cdots & \mu_{1N}^{tr} \\ \vdots & \cdots & \vdots & \cdots & \vdots & \cdots \\ \mu_{N1}^{tt} & \cdots & \mu_{NN}^{tt} & \mu_{N1}^{tr} & \cdots & \mu_{NN}^{tr} \\ \mu_{11}^{rt} & \cdots & \mu_{1N}^{rt} & \mu_{11}^{rr} & \cdots & \mu_{1N}^{rr} \\ \vdots & \cdots & \vdots & \cdots & \vdots & \cdots \\ \mu_{N1}^{rt} & \cdots & \mu_{NN}^{rt} & \mu_{N1}^{rr} & \cdots & \mu_{NN}^{rr} \end{pmatrix}, \tag{1.1}$$

which contains four $3N\times 3N$ blocks for translation, $\boldsymbol{\mu}^{tt}$, rotation, $\boldsymbol{\mu}^{rr}$, and translation rotation coupling $\boldsymbol{\mu}^{tr}$, and $\boldsymbol{\mu}^{rt}=(\boldsymbol{\mu}^{tr})^T$, where $N$ is the number of beads. The translational-translational mobility $\boldsymbol{\mu}^{tt}$ is

$$\mu_{ii}^{tt}=\frac{1}{6\pi\eta a}I, \tag{1.2a}$$

$$\mu_{ij}^{tt}=\frac{1}{8\pi\eta r_{ij}}\left[\left(1+\frac{2a^2}{3r_{ij}^2}\right)I+\left(1-\frac{2a^2}{r_{ij}^2}\right)\frac{\boldsymbol{r}_{ij}\otimes\boldsymbol{r}_{ij}}{r_{ij}^2}\right], \qquad i\neq j, \qquad r_{ij}>2a, \tag{1.2b}$$

$$\mu_{ij}^{tt}=\frac{1}{6\pi\eta a}\left[\left(1-\frac{9r_{ij}}{32a}\right)I+\frac{3r_{ij}}{32a}\frac{\boldsymbol{r}_{ij}\otimes\boldsymbol{r}_{ij}}{r_{ij}^2}\right], \qquad i\neq j, \qquad r_{ij}<2a, \tag{1.2c}$$

the rotational degrees of freedom $\boldsymbol{\mu}^{rr}$ is

$$\mu_{ii}^{rr}=\frac{1}{8\pi\eta a^3}I, \tag{1.3a}$$

$$\mu_{ij}^{rr}=-\frac{1}{16\pi\eta r_{ij}^3}\left(I-3\frac{\boldsymbol{r}_{ij}\otimes\boldsymbol{r}_{ij}}{r_{ij}^2}\right), \qquad i\neq j, \quad r_{ij}>2a, \tag{1.3b}$$

$$\mu_{ij}^{rr}=\frac{1}{8\pi\eta a^3}\left[\left(1-\frac{27}{32}\frac{r_{ij}}{a}+\frac{5}{64}\frac{r_{ij}^3}{a^3}\right)I+\left(\frac{9}{32}\frac{r_{ij}}{a}-\frac{3}{64}\frac{r_{ij}^3}{a^3}\right)\frac{\boldsymbol{r}_{ij}\otimes\boldsymbol{r}_{ij}}{r_{ij}^2}\right], \quad i\neq j, \quad r_{ij}<2a, \tag{1.3c}$$

finally, the translation-rotational mobility is described by the following tensor:

$$\mu_{ii}^{tr}=\mu_{ii}^{rt}=0, \tag{1.4a}$$

$$\mu_{ij}^{tr}=-\frac{1}{8\pi\eta r_{ij}^2}\boldsymbol{\epsilon}\cdot\frac{\boldsymbol{r}_{ij}}{r_{ij}}, \qquad i\neq j, \qquad r_{ij}>2a, \tag{1.4b}$$

$$\mu_{ij}^{tr}=-\frac{1}{16\pi\eta a^2}\left(\frac{r_{ij}}{a}-\frac{3}{8}\frac{r_{ij}^2}{a^2}\right)\boldsymbol{\epsilon}\cdot\frac{\boldsymbol{r}_{ij}}{r_{ij}}, \quad i\neq j, \qquad r_{ij}<2a, \tag{1.4c}$$