IV International Conference on Computational Methods for Coupled Problems in Science and Engineering
COUPLED PROBLEMS 2011
M. Papadrakakis, E. Oñate and B. Schrefler (Eds)

EFFICIENT FORCE FIELD CALCULATION IN ARTICULATED MULTISCALE MOLECULAR SIMULATIONS

MOHAMMAD POURSINA* AND KURT S. ANDERSON*

*Computational Dynamics Lab (CDL)
Department of Mechanical, Aerospace and Nuclear Engineering
Rensselaer Polytechnic Institute
Troy, NY 12180, USA
e-mail: poursm@rpi.edu, anderk5@rpi.edu

Key words: Force Field, Pseudo-center, Pseudo-inertia Tensor, Multiscale Problems

Abstract. Multiscale simulations of molecular systems such as proteins, DNAs, and RNAs are implemented using models with different resolutions ranging from a fully atomistic model to coarse-grained molecules, up to a continuum level system descriptions. For such simulations, pairwise force calculation is a serious bottleneck which can impose a prohibitive amount of computational load on the simulation if not performed wisely. Herein, a novel method is presented to approximate the resultant force and the associated moment for long-range particle-body and body-body interactions applicable to multiresolution coarse-grained simulation of biopolymers. The resultant moment is due to the fact that the net force does not necessarily act through the center of mass of the body. This moment is neglected in bead-based coarse models which use particle dynamics to form the equations of motion of each large spherical pseudo-atom. The presented method significantly reduces the cost of the force field calculations specially in multiscale models which contain rigid subdomains.

1 INTRODUCTION

Function of most biopolymers such as DNA and RNA is highly related to their structure. As such, modeling and simulation of such systems are performed to predict the associated structure accurately in a timely manner. Such systems with large number of particles ($n \approx 10^6$ [1]) suffer from the cumbersome pairwise force field calculations with the computational complexity of $O(n^2)$ at each time step. Therefore, different algorithms have been developed to efficiently calculate far-field interactions. Ewald summation method applicable to periodic systems [2, 3] is the approach which calculates the long-range field in Fourier space. For non-periodic systems, particle-mesh (PM) and particle-particle particle-mesh (PPPM) techniques perform satisfactorily when the required precision is low and the particles are distributed more or less uniformly [4]-[6]. As the next generation of the fast algorithms, the first tree methods

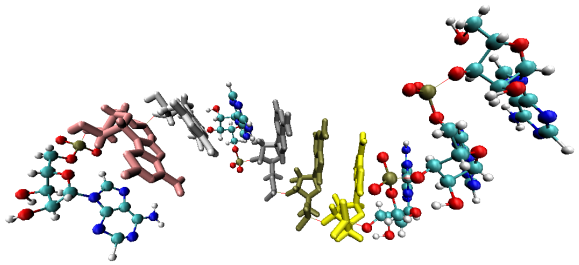

Figure 1: Multiscale modeling of an RNA

[4] presented in [7] and [8] provide the monopole approximation of the long-range field in the system. Using higher order multipole expansion, Fast Multipole Method (FMM) is presented in [9] to approximate the electrostatic field of a group of particles with a computational complexity of $O(n)$. This method is later extended and used to approximate different potential fields for different systems [10]-[13].

Eliminating high frequency modes of motion by considering groups of atoms as rigid or flexible bodies, coarse-grained simulations of biopolymers improve the integration time step. Additionally, they reduce the computational cost associated with pairwise force calculations by ignoring the interactions among particles embedded in rigid regions of the system. This technique may be implemented by replacing different subdomains of the system with rigid or flexible bodies. Using internal coordinates, these regions are connected together via kinematic joints [14]-[16]. Alternatively, coarse-grained modeling may be implemented by considering a group of atoms as a spherical bead, and applying particle dynamics to formulate the equations of motion of each large pseudo-atom [17, 18]. Such systems may also be modeled in the multiscale and/or adaptive [16] framework to capture the dynamics of the system more accurately. These models may contain multiple resolutions ranging from fine scale atomistic domains, coarse-grained macromolecules to continuum level system descriptions.

Herein, we extend the approach used to approximate long-range gravitational force and the associated moment in spacecraft dynamics [19] to the pairwise forces in articulated multiscale simulation of molecular systems. We provide an approximation of the resultant force and the associated moment applied from a particle to a body (pseudo-atom) consisting of many particles. The resultant moment approximated here is due to the fact that the net force does not necessarily act through the center of mass of the body (pseudo-atom). This moment should be considered when the equations of motion are formed in an articulated multibody framework. However, it is neglected in most coarse-grained bead models which use particle dynamics. These approximations can be used to find the long-range interactions between the atoms and rigidified nucleotides of an RNA shown in Fig. 1. We also derive the approximation for the spatial force due to the interactions between particles embedded in two pseudo-atoms (bodies). For the same system shown in Fig. 1, this approximation is applied to find the far-field interactions among the rigidified nucleotides. Herein, multipole and Taylor series expansion coefficients are elaborated and as such, expressed using terms with physical meanings. For instance, we define pseudo-

center and pseudo-inertia tensor for each body. Then, we express the approximations in terms of the location of the pseudo-center and specific elements of the pseudo-inertia tensor of each body. This tensor is calculated for each *rigid* subdomain of the system before starting the simulation. We also show that if the pseudo-center is defined for the subdomain and is selected as the origin of the body-fixed frame, the first (dipole) moment disappears in the force approximation.

2 FORCE ON A SMALL BODY FROM A PARTICLE

Consider particle $\bar{P}$, and body B (not necessarily a rigid body) containing N particles shown in Fig. 2. Any arbitrary particle P_i belonging to B experiences a pairwise force due to its interaction with $\bar{P}$. Herein, we assume that this force is expressed by the following relation

$$\mathbf{F}_{\bar{P}P_i} = \frac{\kappa\bar{\lambda}\lambda_i}{(|\mathbf{r'}_i|)^s}\mathbf{e}_{\mathbf{r'}_i} = \kappa\bar{\lambda}\lambda_i\mathbf{r'}_i(\mathbf{r'}_i^2)^{-\frac{s+1}{2}}, \tag{1}$$

where, λ_i and $\bar{\lambda}$ are the quantities corresponding to the force field, κ is the constant associated with the force field of interest, and s is an integer. In this formula, $\mathbf{e}_{\mathbf{r'}_i}$ is the unit vector from particle $\bar{P}$ to P_i. This general formulation may be used to address the gravitational, Coulombic or London forces. For instance, if one is interested in pairwise forces due to the Coulomb's law, κ is replaced by the Coulomb force constant, λ_i represents the charge of the particle, and s becomes 2. For each body, we define the lumped quantity corresponding to the quantity of interest λ as

$$\Lambda \triangleq \sum_{i=1}^{N} \lambda_i. \tag{2}$$

We also define the "pseudo-center" of the body denoted by C_λ. Position vector of this point with respect to the center of mass (i.e., B^*) is determined by the following relation

$$\mathbf{R}_\lambda = \frac{\sum_{i=1}^{N} \mathbf{R}_i\lambda_i}{\Lambda}, \tag{3}$$

provided that $\Lambda \neq 0$. In the above relation, $\mathbf{R}_i$ is the position vector of the particle (atom) P_i measured from the center of mass of the body. In the following derivations, it is assumed that the origin of the body-fixed frame coincides with the pseudo-center of the body.

Using the following relation based on Fig.2,

$$\mathbf{r'}_i = \mathbf{R} + \mathbf{r}_i, \tag{4}$$

Eq. (1) is rewritten as

$$\mathbf{F}_{\bar{P}P_i} = \kappa\bar{\lambda}\lambda_i(\mathbf{R} + \mathbf{r}_i)(\mathbf{R}^2 + \mathbf{r}_i^2 + 2\mathbf{R}\cdot\mathbf{r}_i)^{-\frac{s+1}{2}}. \tag{5}$$

Introducing the intermediate vector $\mathbf{q}_i$ as

$$\mathbf{q}_i = \frac{\mathbf{r}_i}{R}, \tag{6}$$

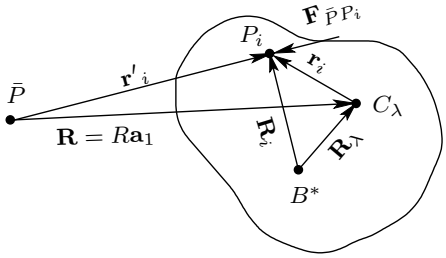

Figure 2: Particle $\bar{P}$ applies the force $\mathbf{F}_{\bar{P}P_i}$ to the particle P_i on body B.

and expressing vector $\mathbf{R}$ as

$$\mathbf{R} = R\mathbf{a}_1, \tag{7}$$

one can rewrite Eq. (5) in the following format

$$\mathbf{F}_{\bar{P}P_i} = \frac{\kappa\bar{\lambda}\lambda_i}{R^s}(\mathbf{a}_1 + \mathbf{q}_i)(1 + \mathbf{q}_i^2 + 2\mathbf{a}_1 \cdot \mathbf{q}_i)^{-\frac{s+1}{2}}. \tag{8}$$

Recalling the binomial series expansion,

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2}x^2 + \frac{n(n-1)(n-2)}{3!}x^2 + ... \quad (|x| < 1), \tag{9}$$

the term $(1 + \mathbf{q}_i^2 + 2\mathbf{a}_1 \cdot \mathbf{q}_i)^{-\frac{s+1}{2}}$ in Eq. (8) is expanded as follows if $|\mathbf{q}_i^2 + 2\mathbf{a}_1 \cdot \mathbf{q}_i| < 1$

$$\begin{aligned}(1 + \mathbf{q}_i^2 &+ 2\mathbf{a}_1 \cdot \mathbf{q}_i)^{-\frac{s+1}{2}} \\ &= 1 - \frac{s+1}{2}(\mathbf{q}_i^2 + 2\mathbf{a}_1 \cdot \mathbf{q}_i) + \frac{(s+1)(s+3)}{8}(\mathbf{q}_i^2 + 2\mathbf{a}_1 \cdot \mathbf{q}_i)^2 \\ &- \frac{(s+1)(s+3)(s+5)}{48}(\mathbf{q}_i^2 + 2\mathbf{a}_1 \cdot \mathbf{q}_i)^3 + ...\end{aligned} \tag{10}$$

Using the expression provided in Eq. (10), the total force experienced by body B due to the pairwise interactions between its own particles and $\bar{P}$ is rewritten as

$$\begin{aligned}\mathbf{F}_{\bar{P}B} &= \frac{\kappa\bar{\lambda}}{R^s}[\sum_{i=1}^{N}\lambda_i\mathbf{a}_1 - \sum_{i=1}^{N}(s+1)\lambda_i(\mathbf{a}_1 \cdot \mathbf{q}_i)\mathbf{a}_1 + \sum_{i=1}^{N}\lambda_i\mathbf{q}_i \\ &- \sum_{i=1}^{N}\frac{(s+1)}{2}\lambda_i\mathbf{q}_i^2\mathbf{a}_1 + \sum_{i=1}^{N}\frac{(s+1)(s+3)}{2}\lambda_i(\mathbf{a}_1 \cdot \mathbf{q}_i)^2\mathbf{a}_1 \\ &- \sum_{i=1}^{N}(s+1)\lambda_i(\mathbf{a}_1 \cdot \mathbf{q}_i)\mathbf{q}_i + ...)].\end{aligned} \tag{11}$$

We elaborate on different terms in the above expression based on their orders with respect to $\frac{|\mathbf{r}_i|}{R}$.

- $O(\frac{|\mathbf{r}_i|}{R})^0$:

$$\frac{\kappa\bar{\lambda}}{R^s}\sum_{i=1}^{N}\lambda_i\mathbf{a}_1=\frac{\kappa\bar{\lambda}}{R^s}\mathbf{a}_1\sum_{i=1}^{N}\lambda_i\overset{(2)}{=}\frac{\kappa\bar{\lambda}\Lambda}{R^s}\mathbf{a}_1 \tag{12}$$

- $O(\frac{|\mathbf{r}_i|}{R})$:

$$-\frac{\kappa\bar{\lambda}(s+1)}{R^{(s+1)}}\mathbf{a}_1\mathbf{a}_1\cdot\sum_{i=1}^{N}\lambda_i\mathbf{r}_i+\frac{\kappa\bar{\lambda}}{R^{(s+1)}}\sum_{i=1}^{N}\lambda_i\mathbf{r}_i \tag{13}$$

Although it is mentioned in [4] that the dipole moment measured from the center of charge (pseudo-center in this paper) vanishes if "the charges are all positive" [4] ($\lambda_i>0$), in the following we show that the dipole (first) moment measured from the pseudo-center (if defined) becomes zero independent of the sign of λ_i

$$\sum_{i=1}^{N}\lambda_i\mathbf{r}_i \;=\; \sum_{i=1}^{N}\lambda_i(\mathbf{R}_i-\mathbf{R}_\lambda)=\sum_{i=1}^{N}\lambda_i\mathbf{R}_i-\mathbf{R}_\lambda\sum_{i=1}^{N}\lambda_i\overset{(2)}{=}\Lambda\mathbf{R}_\lambda-\Lambda\mathbf{R}_\lambda=\mathbf{0}. \tag{14}$$

Consequently, the first order terms disappear if the pseudo-center is defined as the origin of the body-fixed frame.

- $O(\frac{|\mathbf{r}_i|}{R})^2$:

$$\begin{aligned}\frac{\kappa\bar{\lambda}}{R^{(s+2)}}[-\frac{(s+1)}{2}\mathbf{a}_1\sum_{i=1}^{N}\lambda_i\mathbf{r}_i^2 \;&+\; \frac{(s+1)(s+3)}{2}\mathbf{a}_1\mathbf{a}_1\cdot\sum_{i=1}^{N}\lambda_i\mathbf{r}_i\mathbf{r}_i\cdot\mathbf{a}_1\\ &-\; (s+1)\mathbf{a}_1\cdot\sum_{i=1}^{N}\lambda_i\mathbf{r}_i\mathbf{r}_i].\end{aligned} \tag{15}$$

To simplify the above expression, we define the "pseudo-inertia" tensor for body B associated with the quantity λ with respect to its own pseudo-center as

$$\mathcal{I}_\lambda^{B/C_\lambda}\triangleq\sum_{i=1}^{N}(\mathcal{U}\mathbf{r}_i^2-\mathbf{r}_i\mathbf{r}_i)\lambda_i, \tag{16}$$

where $\mathcal{U}$ denotes the identity tensor. This tensor represents the tensor of the moment of inertia (second moment) of the body if one studies the gravitational force [19]. For the Coulombic force, this tensor turns out to be the quadrupole moment tensor [20]. Defining the trace of the pseudo-inertia tensor as

$$tr(\mathcal{I}_\lambda^{B/C_\lambda})=2\sum_{i=1}^{N}\lambda_i\mathbf{r}_i^2\Longrightarrow\sum_{i=1}^{N}\lambda_i\mathbf{r}_i^2=\frac{1}{2}tr(\mathcal{I}_\lambda^{B/C_\lambda}), \tag{17}$$

and using the following property

$$\sum_{i=1}^{N} \lambda_i \mathbf{r}_i \mathbf{r}_i = \frac{tr(\mathcal{I}_\lambda^{B/C_\lambda})}{2} \mathcal{U} - \mathcal{I}_\lambda^{B/C_\lambda}, \tag{18}$$

the second order terms are simplified as

$$\frac{\kappa \bar{\lambda}}{R^{(s+2)}} [-\frac{(s+1)}{4} tr(\mathcal{I}_\lambda^{B/C_\lambda}) \mathbf{a}_1 + \frac{(s+1)(s+3)}{2} \mathbf{a}_1 \mathbf{a}_1 \cdot (\frac{tr(\mathcal{I}_\lambda^{B/C_\lambda})}{2} \mathcal{U} - \mathcal{I}_\lambda^{B/C_\lambda}) \cdot \mathbf{a}_1$$
$$-(s+1) \mathbf{a}_1 \cdot (\frac{tr(\mathcal{I}_\lambda^{B/C_\lambda})}{2} \mathcal{U} - \mathcal{I}_\lambda^{B/C_\lambda})]. \tag{19}$$

Substituting Eqns. (12), (13), and (19) into Eq. (11), the net force applied to the body is expressed as

$$\begin{aligned} \mathbf{F}_{\bar{P}B} &= \frac{\kappa \bar{\lambda}}{R^s} \{\Lambda \mathbf{a}_1 + [\frac{s(s+1)}{4R^2} tr(\mathcal{I}_\lambda^{B/C_\lambda}) - \frac{(s+1)(s+3)}{2R^2} \mathbf{a}_1 \cdot \mathcal{I}_\lambda^{B/C_\lambda} \cdot \mathbf{a}_1] \mathbf{a}_1 \\ &+ \frac{s+1}{R^2} \mathbf{a}_1 \cdot \mathcal{I}_\lambda^{B/C_\lambda} + O(\frac{\mathbf{r}}{R})^3\}, \end{aligned} \tag{20}$$

where $\mathbf{r}$ is the position vector of a generic point on B with respect to the pseudo-center of the body. If the particle $\bar{P}$ is far enough from the pseudo-center of the body such that the largest distance from the pseudo-center to the particles embedded in body B is smaller than the distance between $\bar{P}$ and C_λ, i.e., $\max_{i \in B} |\mathbf{r}_i| << R$, one can ignore the third and higher order terms in Eq. (20). Additionally, introducing a dextral, orthogonal set of unit vectors, $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$, and defining the elements of the pseudo-inertia matrix in $\mathbf{a}$-basis as

$$I_{ij} = \mathbf{a}_i \cdot \mathcal{I}_\lambda^{B/C_\lambda} \cdot \mathbf{a}_j \quad (i,j = 1,2,3), \tag{21}$$

one arrives at the following approximation for the resultant force

$$\begin{aligned} \tilde{\mathbf{F}}_{\bar{P}B} &= \frac{\kappa \bar{\lambda}}{R^s} \{\Lambda \mathbf{a}_1 + [\frac{s(s+1)}{4R^2} tr(\mathcal{I}_\lambda^{B/C_\lambda}) - \frac{(s+1)(s+3)}{2R^2} I_{11}] \mathbf{a}_1 \\ &+ \frac{s+1}{R^2} (I_{11} \mathbf{a}_1 + I_{21} \mathbf{a}_2 + I_{31} \mathbf{a}_3)\}. \end{aligned} \tag{22}$$

The above equation represents the second order multipole approximation of the force applied from particle $\bar{P}$ to body B. The first term shows the interaction between the particle and the body in which the whole body is treated as a particle located at its pseudo-center with the lumped quantity Λ. Since the origin of the body-fixed frame is located at its pseudo-center, the first moment does not appear in the approximate force. Further, the trace of the pseudo-inertia tensor which appears in this expression is an invariant quantity for *rigid* superatoms. In other words, it does not change when the orientation and location of the rigid body changes within the

course of the simulation. As such, once this term is calculated, there is no need to update it. The pseudo-inertia tensor is also a constant matrix for the rigid body if expressed in its body-basis. Therefore, if this tensor is calculated for a rigid subdomain of the system at some time either before or during the simulation, there is no additional cost associated with forming or using this dyadic during the course of the simulation. It is only necessary to monitor the superatom location and orientation to update this tensor at each time step.

Since the pseudo-center is not defined (see Eq. (3)) for a body with zero lumped quantity Λ, the center of mass of the body (subdomain) is considered as the origin of the body-fixed frame to derive the above equations. As such, the pseudo-inertia tensor used in Eq. (22) is defined about B^*. Since the origin of the body-fixed frame is located at the center of mass of the body rather than the pseudo-center, unlike the previous derivations, the first moment is not zero. For such a system, using the relation $\sum_{\substack{i=1\\i\neq j}}^{N}\lambda_i = -\lambda_j$ from Eq. (2), one can rewrite the first moment measured from the center of mass of the body as

$$\sum_{i=1}^{N}\lambda_i\mathbf{R}_i = \sum_{\substack{i=1\\i\neq j}}^{N}(\lambda_i\mathbf{R}_i) + \lambda_j\mathbf{R}_j = \sum_{\substack{i=1\\i\neq j}}^{N}\lambda_i\mathbf{R}_i - \mathbf{R}_j\sum_{\substack{i=1\\i\neq j}}^{N}\lambda_i = \sum_{\substack{i=1\\i\neq j}}^{N}\lambda_i(\mathbf{R}_i-\mathbf{R}_j), \tag{23}$$

which is effectively the first moment measured from the reference point j. Since j is an arbitrary point of the body, this relation demonstrates that if the pseudo-center is not defined for the subdomain, the first moment is constant regardless of the choice of the origin. Consequently, when the lumped quantity of the pseudo-atom is zero, it is necessary to consider its origin-independent first moment in Eq. (22). Further, this term becomes time-invariant for rigid subdomains of the system.

3 FORCE ON A SMALL BODY FROM A SMALL BODY

Consider bodies B and $\bar{B}$ shown in Fig. 3 containing N and $\bar{N}$ particles, respectively. Each body experiences a resultant force due to the pairwise interactions between particles $\{P_i\}_{i=1}^{N}$ belonging to B, and $\{\bar{P}_j\}_{j=1}^{\bar{N}}$ embedded in $\bar{B}$. Summing over the low order approximation of the resultant forces applied to B by particles $\bar{P}_j$ on $\bar{B}$ from Eq. (22), one arrives at the approximate net force applied to body B from $\bar{B}$ as

$$\begin{aligned}\tilde{\mathbf{F}}_{\bar{B}B} &= \sum_{j=1}^{\bar{N}}\frac{\kappa\Lambda\lambda_j}{\bar{R}_j^s}\bar{\mathbf{a}}_1^j + \frac{\kappa\lambda_j}{\bar{R}_j^s}\sum_{j=1}^{\bar{N}}\{[\frac{s(s+1)}{4\bar{R}_j^2}tr(\mathcal{I}_\lambda^{B/C_\lambda})\\ &- \frac{(s+1)(s+3)}{2\bar{R}_j^2}\bar{\mathbf{a}}_1^j\cdot\mathcal{I}_\lambda^{B/C_\lambda}\cdot\bar{\mathbf{a}}_1^j]\bar{\mathbf{a}}_1^j + \frac{s+1}{\bar{R}_j^2}\bar{\mathbf{a}}_1^j\cdot\mathcal{I}_\lambda^{B/C_\lambda}\},\end{aligned} \tag{24}$$

where $\bar{R}_j$ denotes the distance from $\bar{P}_j$ to the pseudo-center of body B, and $\bar{\mathbf{a}}_1^j$ is the corresponding unit vector.

We initially elaborate on the first summation in the above equation. Based on the geometry

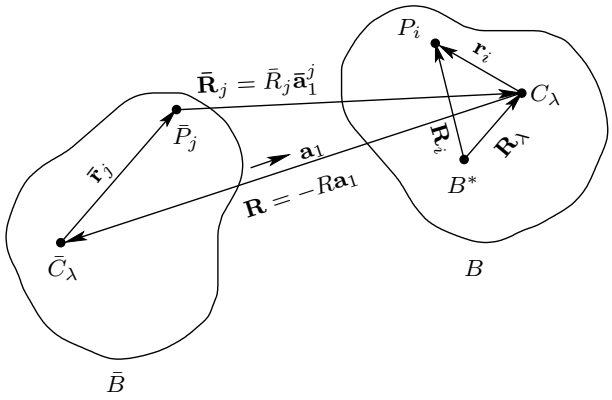

Figure 3: Body $\bar{B}$ applies a resultant force to body B due to the pairwise interaction between the particles belonging to different bodies.

shown in Fig. 3, the term $\frac{\bar{\mathbf{a}}_1^j}{\bar{R}_j^s}$ can be replaced by the following relation

$$\frac{\bar{\mathbf{a}}_1^j}{\bar{R}_j^s} = \bar{\mathbf{R}}_j(\bar{\mathbf{R}}_j^2)^{-\frac{s+1}{2}} = -(\mathbf{R}+\bar{\mathbf{r}}_j)(\mathbf{R}^2+\bar{\mathbf{r}}_j^2+2\mathbf{R}\cdot\bar{\mathbf{r}}_j)^{-\frac{s+1}{2}}, \tag{25}$$

where $\mathbf{R}$ is the position vector of the pseudo-center of body $\bar{B}$ relative to the pseudo-center of body B which is written as

$$\mathbf{R} = -R\mathbf{a}_1. \tag{26}$$

Introducing the intermediate vector $\bar{\mathbf{q}}_j = -\frac{\bar{\mathbf{r}}_j}{R}$, Eq. (25) becomes

$$\frac{\bar{\mathbf{a}}_1^j}{\bar{R}_j^s} = \frac{1}{R^s}(\mathbf{a}_1+\bar{\mathbf{q}}_j)(1+\bar{\mathbf{q}}_j^2+2\mathbf{a}_1\cdot\bar{\mathbf{q}}_j)^{-\frac{s+1}{2}}. \tag{27}$$

We replace the first summation of Eq. (24) with the above expression and expand the term $(1+\bar{\mathbf{q}}_j^2+2\mathbf{a}_1\cdot\bar{\mathbf{q}}_j)^{-\frac{s+1}{2}}$ using the binomial expansion described in section 2. The zeroth order terms in $\frac{\bar{\mathbf{r}}_j}{R}$ are treated the same as those provided in Eq. (12). Similar to the results provided for Eq. (13), the first order terms in $\frac{\bar{\mathbf{r}}_j}{R}$ disappear since the pseudo-center coincides with the origin of the body-fixed frame. The second order terms are even functions of $\bar{\mathbf{q}}_j = -\frac{\bar{\mathbf{r}}_j}{R}$. As such, the negative sign used in the definition of $\bar{\mathbf{q}}_j$ disappears. Therefore, this vector in the second order terms is treated exactly the same as $\mathbf{q}_i$ in Eq. (15). Finally, the first term of Eq. (24) is approximated by

$$\begin{aligned}\sum_{j=1}^{\bar{N}} \frac{\kappa\Lambda\lambda_j}{\bar{R}_j^s}\bar{\mathbf{a}}_1^j &\approx \frac{\kappa\Lambda\bar{\Lambda}}{R^s}\mathbf{a}_1 + \frac{\kappa\Lambda}{R^s}\{[\frac{s(s+1)}{4R^2}tr(\bar{\mathcal{I}}_\lambda^{\bar{B}/\bar{C}_\lambda}) \\ &- \frac{(s+1)(s+3)}{2R^2}\mathbf{a}_1\cdot\bar{\mathcal{I}}_\lambda^{\bar{B}/\bar{C}_\lambda}\cdot\mathbf{a}_1]\mathbf{a}_1 + \frac{s+1}{R^2}\mathbf{a}_1\cdot\bar{\mathcal{I}}_\lambda^{\bar{B}/\bar{C}_\lambda}\},\end{aligned} \tag{28}$$

where $\bar{\mathcal{I}}_{\lambda}^{\bar{B}/\bar{C}_{\lambda}}$ is the pseudo-inertia tensor of body $\bar{B}$ about its pseudo-center, and the lumped quantity of body $\bar{B}$ is defined as $\bar{\Lambda} \triangleq \sum_{j=1}^{\bar{N}} \bar{\lambda}_j$.

In the second summation of Eq. (24), $\bar{R}$ and $\bar{\mathbf{a}}_1^j$ may be replaced by R and $\mathbf{a}_1$, respectively, since this summation involves the terms of second or higher degree in $|\mathbf{r}_i|$, so that no terms of interest for the purpose at hand are lost through this replacement. Defining the elements of the pseudo-inertia tensors of the bodies in $\mathbf{a}$-basis, this relation is expressed in terms of the elements of the pseudo-inertia tensor as

$$\begin{aligned}\tilde{\mathbf{F}}_{\bar{B}B} &= \frac{\kappa\Lambda\bar{\Lambda}}{R^s}\mathbf{a}_1 + \frac{\kappa\Lambda}{R^s}\{[\frac{s(s+1)}{4R^2}tr(\bar{\mathcal{I}}_{\lambda}^{\bar{B}/\bar{C}_{\lambda}}) - \frac{(s+1)(s+3)}{2R^2}\bar{I}_{11}]\mathbf{a}_1 \\ &+ \frac{s+1}{R^2}(\bar{I}_{11}\mathbf{a}_1 + \bar{I}_{21}\mathbf{a}_2 + \bar{I}_{31}\mathbf{a}_3)\} + \frac{\kappa\bar{\Lambda}}{R^s}\{[\frac{s(s+1)}{4R^2}tr(\mathcal{I}_{\lambda}^{B/C_{\lambda}}) \\ &- \frac{(s+1)(s+3)}{2R^2}I_{11}]\mathbf{a}_1 + \frac{s+1}{R^2}(I_{11}\mathbf{a}_1 + I_{21}\mathbf{a}_2 + I_{31}\mathbf{a}_3)\}. \end{aligned} \quad (29)$$

The approximation provided in Eq. (29) is valid if the distance between the pseudo-centers of bodies B and $\bar{B}$ is greater than the distance between the pseudo-center of each body and the corresponding farthest particle, i.e., $\max_{i\in B}|\mathbf{r}_i| << R$ and $\max_{j\in\bar{B}}|\bar{\mathbf{r}}_j| << R$. The symmetry observed in the net force properly implies that the provided approximation does not violate Newton's third law of motion.

4 MOMENT ON A SMALL BODY FROM A PARTICLE

Since the resultant force calculated in section 2 does not generally act through the center of mass of the body, it creates a moment about B^*. Based on the geometry shown in Fig. 2, the resultant moment about B^* due to the interaction between $\bar{P}$ and P_i is expressed by the following cross product

$$\mathbf{M}_{\bar{P}P_i}^{B^*} = \mathbf{R}_i \times \mathbf{F}_{\bar{P}P_i}. \quad (30)$$

According to Fig. 2, and knowing that both $\mathbf{r'}_i$ and $\mathbf{F}_{\bar{P}P_i}$ are collinear vectors, this moment becomes

$$\mathbf{M}_{\bar{P}P_i}^{B^*} = (\mathbf{R}_{\lambda} - \mathbf{R}) \times \mathbf{F}_{\bar{P}P_i} + \underbrace{\mathbf{r'}_i \times \mathbf{F}_{\bar{P}P_i}}_{\mathbf{0}}. \quad (31)$$

As such, body B experiences the following moment about its center of mass due to the interactions between its own particles and $\bar{P}$

$$\mathbf{M}_{\bar{P}B}^{B^*} = \sum_{i=1}^{N}(\mathbf{R}_{\lambda} - \mathbf{R}) \times \mathbf{F}_{\bar{P}P_i} = (\mathbf{R}_{\lambda} - \mathbf{R}) \times \sum_{i=1}^{N}\mathbf{F}_{\bar{P}P_i} = (\mathbf{R}_{\lambda} - \mathbf{R}) \times \mathbf{F}_{\bar{P}B}. \quad (32)$$

Substituting $\mathbf{R}$ from Eq. (7) into the above equation, using the approximate force from Eq. (20), and defining the elements of the pseudo-inertia tensor in $\mathbf{a}$-basis, the approximate moment about

the center of mass of the body is expressed as

$$\begin{aligned}\tilde{\mathbf{M}}^{B^*}_{\bar{P}B} &= \frac{\kappa\bar{\lambda}}{R^s}\mathbf{R}_\lambda \times \{\Lambda\mathbf{a}_1 + [\frac{s(s+1)}{4R^2}tr(\mathcal{I}^{B/C_\lambda}_\lambda) - \frac{(s+1)(s+3)}{2R^2}I_{11}]\mathbf{a}_1 \\ &+ \frac{s+1}{R^2}(I_{11}\mathbf{a}_1 + I_{21}\mathbf{a}_2 + I_{31}\mathbf{a}_3)\} - \frac{\kappa\bar{\lambda}(s+1)}{R^{(s+1)}}(I_{21}\mathbf{a}_3 - I_{31}\mathbf{a}_2). \end{aligned} \quad (33)$$

In the above equation, if the pseudo-center and the center of mass of the body coincide, i.e., $\mathbf{R}_\lambda = \mathbf{0}$, the last term only contributes to the moment applied to body B. In this case, if $\mathbf{a}_1$ is aligned with one of the principal axes of the pseudo-inertia tensor of body B, the approximate moment formulation provides a zero value. As such, the analyst may use the exact calculations or higher order approximation to find the moment.

5 MOMENT ON A SMALL BODY FROM A SMALL BODY

Since the resultant force applied to body B from body $\bar{B}$ does not necessarily pass through the center of mass of body B, it creates a moment about B^*. As such, the resultant moment can be approximated as a summation over the approximate moments applied by each particle $\bar{P}_j$ on $\bar{B}$ to body B as

$$\begin{aligned}\tilde{\mathbf{M}}^{B^*}_{\bar{B}B} &= \sum_{j=1}^{\bar{N}} \frac{\kappa\lambda_j\Lambda}{\bar{R}^s_j}\mathbf{R}_\lambda \times \bar{\mathbf{a}}^j_1 + \sum_{j=1}^{\bar{N}} \frac{\kappa\lambda_j}{\bar{R}^s_j}\mathbf{R}_\lambda \times \{[\frac{s(s+1)}{4\bar{R}^2_j}tr(\mathcal{I}^{B/C_\lambda}_\lambda) \\ &- \frac{(s+1)(s+3)}{2\bar{R}^2_j}\bar{\mathbf{a}}^j_1 \cdot \mathcal{I}^{B/C_\lambda}_\lambda \cdot \bar{\mathbf{a}}^j_1]\bar{\mathbf{a}}^j_1 + \frac{s+1}{\bar{R}^2_j}\bar{\mathbf{a}}^j_1 \cdot \mathcal{I}^{B/C_\lambda}_\lambda\} \\ &- \sum_{j=1}^{\bar{N}} \frac{\kappa\lambda_j(s+1)}{\bar{R}^{(s+1)}_j}\bar{\mathbf{a}}^j_1 \times (\bar{\mathbf{a}}^j_1 \cdot \mathcal{I}^{B/C_\lambda}_\lambda). \end{aligned} \quad (34)$$

The first summation can be expanded exactly the same as the manipulation conducted in section 3. Similarly, since the terms in the second and third summations are second or higher orders in $|\bar{\mathbf{r}}_j|$, we may replace $\bar{R}$ and $\bar{\mathbf{a}}^j_1$ by R and $\mathbf{a}_1$, respectively. Defining the elements of the pseudo-inertia tensors of the bodies in $\mathbf{a}$-basis, the approximate moment about the center of mass of body B from $\bar{B}$ due to the pairwise interactions between the particles embedded in B and $\bar{B}$ is expressed as

$$\begin{aligned}&\tilde{\mathbf{M}}^{B^*}_{\bar{B}B} = \frac{\kappa\Lambda\bar{\Lambda}}{R^s}\mathbf{R}_\lambda \times \mathbf{a}_1 \\ &+\frac{\kappa\Lambda}{R^s}\mathbf{R}_\lambda \times \{[\frac{s(s+1)}{4R^2}tr(\bar{\mathcal{I}}^{\bar{B}/\bar{C}_\lambda}_\lambda) - \frac{(s+1)(s+3)}{2R^2}\bar{I}_{11}]\mathbf{a}_1 + \frac{s+1}{R^2}(\bar{I}_{11}\mathbf{a}_1 + \bar{I}_{21}\mathbf{a}_2 + \bar{I}_{31}\mathbf{a}_3)\} \\ &+\frac{\kappa\bar{\Lambda}}{R^s}\mathbf{R}_\lambda \times \{[\frac{s(s+1)}{4R^2}tr(\mathcal{I}^{B/C_\lambda}_\lambda) - \frac{(s+1)(s+3)}{2R^2}I_{11}]\mathbf{a}_1 + \frac{s+1}{R^2}(I_{11}\mathbf{a}_1 + I_{21}\mathbf{a}_2 + I_{31}\mathbf{a}_3)\} \\ &-\frac{\kappa\bar{\Lambda}(s+1)}{R^{(s+1)}}(I_{21}\mathbf{a}_3 - I_{31}\mathbf{a}_2). \end{aligned} \quad (35)$$

In the above equation, if the pseudo-center and center of mass of body B coincide, only the last term survives and contributes to the moment. In this case, if $\mathbf{a}_1$ is aligned with one of the principal axes of the pseudo-inertia tensor of body B, the moment becomes zero. Consequently, either the exact moment calculation may be used to find the resultant moment or the moment is approximated considering higher order terms.

6 CONCLUSIONS

A novel method to approximate the resultant force and moment due to the long-range particle-body and body-body interactions in Cartesian coordinates has been presented. The effective moment is due to the fact the resultant force does not necessarily act through the center of mass of the body. In this low order multipole approximation, for each body of the system, a pseudo-center and pseudo-inertia tensor have been defined. Using the pseudo-center of the body (if defined) as the origin of the body-fixed frame, the first (dipole) moment disappears in the force approximation. In this derivation, the quadrupole terms have been elaborated and expressed in terms of the elements of the pseudo-inertia tensor (qurdaupole moment tensor). This matrix is constant for each rigid body (subdomain) if expressed in its own body basis. As such, it is formed in the preprocessing step, and there is no additional cost associated with forming this tensor during the course of the simulation.

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