# A Force Evaluation Free Method to *N*-Body Problems: Binary Interaction Approximation

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**Abstract**

We recently proposed the binary interaction approximation (BIA) to *N*-body problems, which, in principle, excludes the interparticle force evaluation if the exact solutions are known for the corresponding two-body problems such as the Coulombic and gravitational interactions. In this article, a detailed introduction to the BIA is given, including the error analysis to give the expressions for the approximation error in the total angular momentum and the total energy of the entire system. It is shown that, although the energy conservation of the BIA scheme is worse than the 4th order Hermite integrator (HMT4) for similar elapsed, or the wall-clock times, the individual errors in position and in velocity are much better than HMT4. The energy error correction scheme to the BIA is also introduced that does not deteriorates the individual errors in position and in velocity. It is suggested that the BIA scheme is applicable to the tree method, the particle-mesh (PM), and the particle-particle-particle-mesh (PPPM) schemes simply by replacing the force evaluation and the conventional time integrator with the BIA scheme.

*Keywords:* *N*-body problem, binary interaction approximation (BIA), error analysis, energy error correction, pair-wise variable step size, parallel computation, tree method, PPPM.

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## 1. Introduction

In an isolated $N$-body system, the equation of motion for the $i$-th particle at a position $\boldsymbol{r}_i$ with a momentum $\boldsymbol{p}_i = m_i \boldsymbol{v}_i$ is as follows:

$$\frac{\mathrm{d}\boldsymbol{p}_i}{\mathrm{d}t} = \sum_{j \neq i}^{N} \boldsymbol{F}_{ij} \tag{1}$$

where $\boldsymbol{F}_{ij} = \boldsymbol{F}_{ij}(\boldsymbol{r}_i, \boldsymbol{r}_j)$ stands for the interparticle force on the $i$-th particle due to $j$-th particle at a position $\boldsymbol{r}_j$.

When $N \geq 3$, it is well known that no exact/analytical solution can be obtained, and one should be content with approximated solutions using one of numerical integration methods. In principle, to arbitrary error levels the numerical solution can be found [1] if one uses the arbitrary-precision arithmetic. However, it is practically impossible for the huge number of particles, i.e. $N \ggg 1$, since the number of force calculations on the right hand side of Eq. (1) is in proportion to $N^2$. Moreover, the number of time steps tend to increase with increasing $N$, thus the total CPU time should scale as $\sim N^{2+0.3}$-$N^{2+1.3}$.

In order to reduce the CPU time, efforts have been made to use parallel computers, and/or to develop special purpose hardware to calculate interparticle forces, e.g. the GRAvity PipE (GRAPE) project [2], [3].

The efficient and fast algorithms to calculate inter-particle forces include the tree method [4], [5], the fast multipole expansion method (FMM) and the particle-mesh Ewalt (PPPM) method [6]. These methods reduce the effective number of particles and thus force calculations from $O\left(N^2\right)$ to $O(N \ln N)$ or $O(N)$, which make the integration of Eq. (1) much faster than the conventional schemes of order of $N^2$.

The author has recently developed the binary interaction approximation (BIA) to $N$-body problems, which removes the necessity of force evaluation in principle, if the exact solutions are known for the corresponding two-body problems such as the Coulombic and gravitational interactions. The first application of the BIA to two dimensional Coulomb interactions is found in Ref. [7]. In this paper, we will give the theoretical framework of the BIA scheme and its error analysis in Section 2 with Appendix A, and apply the BIA to two- and three-dimensional Coulomb and gravitational $N$-body systems in Section 3. The applicability of the BIA to the PPPM method is suggested in the last Section 4.

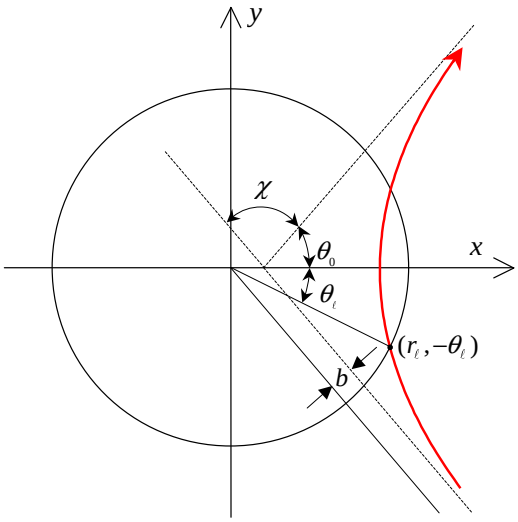


Figure 1: Unperturbed relative trajectory $r = r(\theta)$ in an orbital plane. The scattering center is at the origin. An impact parameter is $b = b_0 \tan\theta_0$.

## 2. BIA: Binary Interaction Approximation to *N*-body problems

As shown in Fig. 1 which depicts the relative motion of the particle pair $i$ and $j$ in the center of mass coordinate system, the scattering angle, $\chi \equiv \pi - 2\theta_0$, is given by $b = b_0 \tan\theta_0$, where $b$ is the impact parameter, $b_0$ corresponds to $\chi = \pi/2$ scattering, and $g_0$ the initial relative speed at $r = r(\theta = -\theta_0) = \infty$. Here $\mu \equiv m_i m_j/(m_i + m_j)$ is the reduced mass. In the case of charged particle systems, $b_0$ is given by

$$b_0 \equiv \frac{q_i q_j}{4\pi\varepsilon_0 \mu g_0^2},$$

and for gravitational systems

$$b_0 \equiv -\frac{\mathcal{G} m_i m_j}{\mu g_0^2} = -\frac{\mathcal{G}\left(m_i + m_j\right)}{g_0^2},$$

where $\mathcal{G}$ is the gravitational constant.

In the binary system, i.e. $N = 2$ in Eq. (1), with an impact parameter $b = b_0 \tan\theta_0 = b_0 \cot\frac{\chi}{2}$, a typical velocity change $\Delta g$ in the relative velocity is given

by

$$\Delta g = 2g_0 \sin\frac{\chi}{2} \sim \chi g_0 \sim \epsilon g_0, \tag{2}$$

since, on the average, $b$ for a test particle is $\langle b\rangle \sim \Delta\ell$ against its closest field particle and $\epsilon \equiv b_0/\Delta\ell \sim \chi$ where $\Delta\ell$ is the average interparticle separation.

In $N$-body systems with $\epsilon \ll 1$, such as the fusion plasmas, Eq. (2) suggests that three-or-more body interactions can be ignored since they are of the order of $\epsilon^2 \lll 1$ and seldom occur due to low density. It should be noted that the Debye lengths $\lambda_{\rm D}$ in fusion plasmas generally satisfy $\lambda_{\rm D} \gg \Delta\ell$, thus typical binary interaction is characterized by the nondimensional parameter $\epsilon$. This parameter is of order of $U/K$, where $U$ and $K$ stand for the potential and kinetic energies.

### *2.1. BIA scheme*

The exact changes $m_i\Delta\boldsymbol{v}_i = \Delta\boldsymbol{p}_i$ in momentum and $\Delta\boldsymbol{r}_i$ in position for solutions to the $N$-body problem given in Eq. (1) are formally given by

$$m_i\Delta\boldsymbol{v}_i = \sum_{j\neq i}^{N}\mu_{ij}\int_0^{\Delta t}\frac{\mathrm{d}\boldsymbol{g}_{ij}(t)}{\mathrm{d}t}\mathrm{d}t, \tag{3}$$

$$m_i\Delta\boldsymbol{r}_i = m_i\boldsymbol{v}_i(0)\,\Delta t + \sum_{j\neq i}^{N}\mu_{ij}\left(\int_0^{\Delta t}\frac{\mathrm{d}\boldsymbol{r}_{ij}(t)}{\mathrm{d}t}\mathrm{d}t - \boldsymbol{g}_{ij}(0)\,\Delta t\right), \tag{4}$$

during a time interval of $\Delta t$, where $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$ stands for the relative position, $\boldsymbol{g}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$ the relative velocity, and $\mu_{ij} = m_im_j/(m_i + m_j)$ the reduced mass.

The equation of relative motion for the charged particle pair $(i, j)$ in an $N$-body system used by the binary interaction approximation, the BIA, is

$$\mu_{ij}\frac{\mathrm{d}\boldsymbol{g}_{ij}}{\mathrm{d}t} = \frac{q_iq_j}{4\pi\varepsilon_0}\frac{\boldsymbol{r}_{ij}}{r_{ij}^3}. \tag{5}$$

In the BIA scheme, the above equation is integrated numerically or analytically, completely ignoring the other particles, from $t = 0$ to $t = \Delta t$ to give $\Delta\boldsymbol{r}_{ij} \equiv \boldsymbol{r}_{ij}(\Delta t) - \boldsymbol{r}_{ij}(0)$ and $\Delta\boldsymbol{g}_{ij} \equiv \boldsymbol{g}_{ij}(\Delta t) - \boldsymbol{g}_{ij}(0)$. The total number of integration is ${}_N\mathrm{C}_2 = N(N-1)/2$ for an $N$-body problem. The individual changes, during an arbitrary interval $\Delta t$, in position $\Delta\boldsymbol{r}_i$ and velocity $\Delta\boldsymbol{v}_i$ of the $i$–th particle are as follows

$$m_i\Delta\boldsymbol{r}_i = m_i\boldsymbol{v}_i\Delta t + \sum_{j\neq i}^{N}\mu_{ij}\left(\Delta\boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t\right), \tag{6}$$

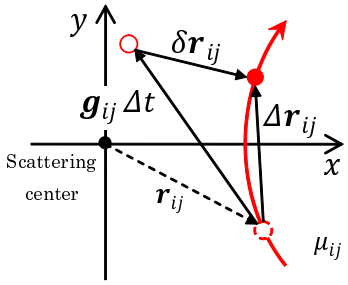


Figure 2: Relative motion of the BIA scheme for the particle pair of $(i, j)$ in their orbital plane. The exact motion is along the curved line (in red). If there is no interaction, the change in position is $\boldsymbol{g}_{ij}\Delta t$ during a time interval of $\Delta t$.

$$m_i \Delta \boldsymbol{v}_i \quad = \quad \sum_{j \neq i}^{N} \mu_{ij} \Delta \boldsymbol{g}_{ij}, \tag{7}$$

for $i = 1, 2, \cdots, N$. Hereafter we will use the notations $\boldsymbol{r}_i$, $\boldsymbol{v}_i$, $\boldsymbol{g}_{ij}$, $\cdots$, for their initial values $\boldsymbol{r}_i(0)$, $\boldsymbol{v}_i(0)$, $\boldsymbol{g}_{ij}(0)$, $\cdots$. Note that the term within the parentheses on the right hand side of Eq. (6), i.e. $\Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t \equiv \delta \boldsymbol{r}_{ij}$ as shown in Fig. 2, vanishes when the interaction between the pair $(i, j)$ vanishes. In other words, the BIA scheme is exact for free particles, in which every $\Delta \boldsymbol{v}_i = 0$, and consequently $\Delta \boldsymbol{r}_i = \boldsymbol{v}_i \Delta t$, for arbitrary $\Delta t$.

It should be noted that each relative motion is restricted in respective orbital plane, thus the BIA requires the calculation of $\Delta \boldsymbol{r}_{ij}$ and $\Delta \boldsymbol{g}_{ij}$ in two dimensions perpendicular to the initial angular momentum $\boldsymbol{L}_{ij} = \boldsymbol{r}_{ij} \times \boldsymbol{p}_{ij}$. In the case of $\boldsymbol{L}_{ij} = \boldsymbol{0}$, the relative motion is further reduced to one dimensional.

### *2.2. Consistency of the BIA scheme*

In the limit of $\Delta t \to 0$, Eq. (6) becomes as

$$\lim_{\Delta t \to 0} \frac{\Delta \boldsymbol{r}_i}{\Delta t} = \boldsymbol{v}_i + \frac{1}{m_i} \sum_{j \neq i}^{N} \mu_{ij} \lim_{\Delta t \to 0} \left( \frac{\Delta \boldsymbol{r}_{ij}}{\Delta t} - \boldsymbol{g}_{ij} \right) = \boldsymbol{v}_i, \tag{8}$$

and similarly Eq. (7) becomes in the same limit as

$$\lim_{\Delta t \to 0} \frac{\Delta \boldsymbol{v}_i}{\Delta t} = \frac{1}{m_i} \sum_{j \neq i}^{N} \mu_{ij} \lim_{\Delta t \to 0} \frac{\Delta \boldsymbol{g}_{ij}}{\Delta t} = \frac{1}{m_i} \sum_{j \neq i}^{N} \boldsymbol{F}_{ij}, \tag{9}$$

which reproduces the original equation of motion given by Eq. (1). In the terminology of the numerical analysis, the BIA scheme with the properties of Eqs. (8) and (9) is said to be consistent.

### *2.3. Conservation of invariants in BIA*

The total linear momentum

$$\boldsymbol{P} \equiv \sum_{i=1}^{N} m_i \boldsymbol{v}_i \tag{10}$$

is kept constant with the BIA scheme for arbitrary time interval $\Delta t$, since, from Eq. (7) and by definition $\mu_{ij} = \mu_{ji}$,

$$\Delta \boldsymbol{P} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \mu_{ij} \left( \Delta \boldsymbol{g}_{ij} + \Delta \boldsymbol{g}_{ji} \right) = \boldsymbol{0}. \tag{11}$$

Similarly, the change in the center of mass position of the entire system in the BIA scheme

$$\boldsymbol{R} \equiv \frac{1}{M} \sum_{i=1}^{N} m_i \boldsymbol{r}_i \tag{12}$$

is also exact as follows; by noting $\delta \boldsymbol{r}_{ij} \equiv \Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij} \Delta t$ in Eq. (6), we have

$$\Delta \boldsymbol{R} = \frac{1}{M} \left( \sum_{i=1}^{N} m_i \boldsymbol{v}_i \Delta t + \sum_{i=1}^{N} \sum_{j \neq i}^{N} \mu_{ij} \delta \boldsymbol{r}_{ij} \right) = \boldsymbol{G} \Delta t, \tag{13}$$

where $\boldsymbol{G} \equiv \boldsymbol{P}/M$ and $M = \sum_{i=1}^{N} m_i$ stand for the mass velocity and the total mass of the system, respectively. Here we have used that the double summation over $i$ and $j$ in Eq. (13) vanishes as

$$\sum_{i=1}^{N} \sum_{j \neq i}^{N} \mu_{ij} \delta \boldsymbol{r}_{ij} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \mu_{ij} \left( \delta \boldsymbol{r}_{ij} + \delta \boldsymbol{r}_{ji} \right) = \boldsymbol{0}, \tag{14}$$

since $\delta \boldsymbol{r}_{ji} = -\delta \boldsymbol{r}_{ij}$ by definition.

Other invariants of the $N$-body system, such as the total angular momentum

$$\boldsymbol{L} \equiv \sum_{i=1}^{N} \boldsymbol{r}_i \times m_i \boldsymbol{v}_i = \sum_{i=1}^{N} \boldsymbol{r}_i \times \boldsymbol{p}_i, \tag{15}$$

and the total energy

$$E = K + U = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} U_{ij}\left(\boldsymbol{r}_{ij}\right)$$

include approximation errors in principle, even though corresponding errors for each binary system are all zero, i.e.,

$$\Delta \boldsymbol{L}_{ij} = \left(\boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_{ij}\right) \times \Delta \boldsymbol{p}_{ij} + \Delta \boldsymbol{r}_{ij} \times \boldsymbol{p}_{ij} = \boldsymbol{0}, \tag{16}$$

and

$$\Delta E_{ij} = \left(\boldsymbol{g}_{ij} + \frac{1}{2}\Delta \boldsymbol{g}_{ij}\right) \cdot \Delta \boldsymbol{p}_{ij} + U_{ij}\left(\boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_{ij}\right) - U_{ij}\left(\boldsymbol{r}_{ij}\right) = 0. \tag{17}$$

As will be derived in Appendix A, the approximation errors in the total angular momentum $\Delta \boldsymbol{L}$ and in the total energy $\Delta E$ in the BIA scheme are respectively given by

$$\Delta \boldsymbol{L} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \delta \hat{\boldsymbol{r}}_{ij} \times \Delta \boldsymbol{p}_{ij}, \tag{18}$$

$$\Delta E = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left(\delta \hat{\boldsymbol{g}}_{ij} \cdot \Delta \boldsymbol{p}_{ij} + \delta \hat{U}_{ij}\right), \tag{19}$$

where $\delta \hat{\boldsymbol{r}}_{ij}$, $\delta \hat{\boldsymbol{g}}_{ij}$, and $\delta \hat{U}_{ij}$ have been defined as

$$\delta \hat{\boldsymbol{r}}_{ij} \equiv \sum_{k \neq i,j}^{N} \left(\frac{\mu_{ik} \delta \boldsymbol{r}_{ik}}{m_i} - \frac{\mu_{jk} \delta \boldsymbol{r}_{jk}}{m_j}\right) = \left(\delta \boldsymbol{r}_i - \delta \boldsymbol{r}_j\right) - \delta \boldsymbol{r}_{ij}, \tag{20}$$

$$\delta \hat{\boldsymbol{g}}_{ij} \equiv \sum_{k \neq i,j}^{N} \left(\frac{\mu_{ik} \Delta \boldsymbol{g}_{ik}}{m_i} - \frac{\mu_{jk} \Delta \boldsymbol{g}_{jk}}{m_j}\right) = \left(\Delta \boldsymbol{v}_i - \Delta \boldsymbol{v}_j\right) - \Delta \boldsymbol{g}_{ij}, \tag{21}$$

$$\delta \hat{U}_{ij} \equiv U_{ij}\left(\boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_{ij} + \delta \hat{\boldsymbol{r}}_{ij}\right) - U_{ij}\left(\boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_{ij}\right). \tag{22}$$

Both $\Delta \boldsymbol{L}$ and $\Delta E$ are of the order of $\epsilon^2$, which is the result of three-or-more-body interactions, among particles $i$, $j$ and $k \neq i, j$, which has been ignored in the BIA scheme. Actually, $\delta \hat{\boldsymbol{r}}_{ij} = \boldsymbol{0}$, $\delta \hat{\boldsymbol{g}}_{ij} = \boldsymbol{0}$, and accordingly $\Delta \boldsymbol{L} = \boldsymbol{0}$ and $\Delta E = 0$ when $N = 2$. Thus, the BIA scheme is most appropriate to be applied to $N$-body systems with small $\epsilon \sim U/K \ll 1$, such as typical fusion plasmas with $\epsilon \sim 10^{-7}$.

### 2.4. Estimation of CPU time in BIA

It is well known that the CPU time $\tau_{\rm DIM}^{\rm CPU} = \tau_{\rm DIM}^{\rm CPU}(N)$ required for a conventional direct integration method (DIM) to solve the full set of equation of motion given in Eq. (1) should scale as

$$\tau_{\rm DIM}^{\rm CPU} \propto N^2 \times {\rm O}\left(N^{0.3-1.3}\right) \sim N^{2.3-3.3}, \tag{23}$$

of which $N^2$ for interaction force calculations, and ${\rm O}\left(N^{0.3-1.3}\right)$ for time integration during a given time interval $\Delta t$. On the other hand, with the BIA scheme the CPU time scales as $N^2$ since a set of ${}_N{\rm C}_2 = N(N-1)/2 \propto N^2$ independent two-body equations of motion given in Eq. (5) can be solved with a CPU time scaling $\tau_{\rm BIA}^{\rm CPU} = \tau_{\rm BIA}^{\rm CPU}(N)$ of

$$\tau_{\rm BIA}^{\rm CPU} \propto N^2 \times {\rm O}(2) \sim N^2. \tag{24}$$

## 3. Test Calculations

In order to show the usefulness of the BIA to $N$-body problems with a wide range of the interaction parameter $\epsilon = U/K$, three cases of $\epsilon \ll 1$, $\epsilon \sim 1$, and $2K + U = 0$ are examined in the following subsections. The embedded formula of Runge-Kutta-Fehlberg (RKF) method [8, 9] with an absolute error tolerance of $10^{-16}$ is used as the direct integration method (DIM) in this paper.

### 3.1. Test Calculation I: dilute gas plasma

We will apply the BIA scheme to a high temperature, low density ions of the same species; $T = 10$ keV and $n = 10^{20}$ m$^{-3}$, which can be found in typical fusion plasmas. In this case the nondimensional parameter $\epsilon \sim 3 \times 10^{-7} \ll 1$.

In the following calculation, positions $\boldsymbol{r}_i$ are normalized by the interparticle separation $\Delta\ell \equiv n^{-1/3} \sim 2 \times 10^{-7}$ m, and velocities $\boldsymbol{v}_i$ by the relative thermal speed, $g_{\rm th} = \sqrt{2kT/\mu} \sim 2 \times 10^6$ m/s. This leads to the time be normalized by $\Delta t \equiv \Delta\ell/g_{\rm th} \sim 10^{-13}$ sec, i.e. the time for a particle with the thermal speed $g_{\rm th}$ to travel the average interparticle separation $\Delta\ell \equiv n^{-1/3}$. In this case the equation of motion for the particle pair $(i, j)$ is represented as

$$\frac{{\rm d}\boldsymbol{g}_{ij}}{{\rm d}t} = \epsilon_{ij}\frac{\boldsymbol{r}_{ij}}{r_{ij}^3},$$

for $1 \le i \le N$ and $j \ne i$. The above $N$-body system will be integrated for a normalized time interval of $\Delta t = 1$ for various number of particles $N$. Spatial

distribution function at the time $t = 0$ is assumed to be uniform with the average particle distance being $\Delta\ell$, and the velocity distribution function also be uniform with the average relative speed being the thermal speed of $g_{\rm th}$.

A 1332-body system is integrated for a time interval $\Delta t = \Delta\ell/g_{\rm th}$. Table 1 compares the DIM and the BIA in position, and in velocity, respectively, as well as the number of time steps, $N_{\rm step}$. The subscripts in the first column indicate the particle number whose numerical errors (or strictly speaking, deviations from the DIM) of the BIA are the maximum among 1332 particles. The agreement between the BIA and the DIM is excellent. It should be noted that they are the only numerical results which the BIA scheme calculates, i.e. the number of time steps of the BIA is unity, while that of the DIM (RKF) is 308.

Table 1: Maximum absolute deviations of the BIA from the DIM in the phase space $\boldsymbol{r} = (x, y, z)$ and $\boldsymbol{v} = (u, v, w)$ for $N = 1,332$, at $t = \Delta t$. Subscripts in the first column, e.g., $x_{902}$, stand for the particle number out of $1,332$ particles.

| | BIA | DIM | deviation |
|---|---|---|---|
| $x_{902}$ | 1.08818622505 | 1.08818622504 | 0.00000000001 |
| $y_{967}$ | 3.71489346371 | 3.71489346372 | 0.00000000001 |
| $z_{913}$ | 4.99288579168 | 4.99288579134 | 0.00000000034 |
| $u_{497}$ | 0.06534783380 | 0.06534783357 | 0.00000000023 |
| $v_{961}$ | −0.16174100160 | −0.16174100129 | 0.00000000031 |
| $w_{913}$ | 0.05998355045 | 0.05998355132 | 0.00000000087 |
| $N_{\rm step}$ | 1 | 308 | |

### *3.2. Test Calculation II: plasma oscillations*

Let us consider a three dimensional $N + 1$ body Coulomb problem, in which there are $N$ electrons. Ions are treated as the uniformly distributed immovable neutralizing background with a uniform charge density of $\rho = en_0$, which means the distributed ions constitute the zero-th particle in the BIA scheme. Suppose that the background ions are contained within a sphere of radius $R$ and electrons are moving in the sphere. The resulting electric field $\boldsymbol{E}$ and electrostatic potential $\varphi$, due to the ion distribution, that electrons feel are given by

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{n_0 e\boldsymbol{r}}{3\pi\varepsilon_0},\ \varphi(\boldsymbol{r}) = -\frac{n_0 e r^2}{6\pi\varepsilon_0}. \tag{25}$$

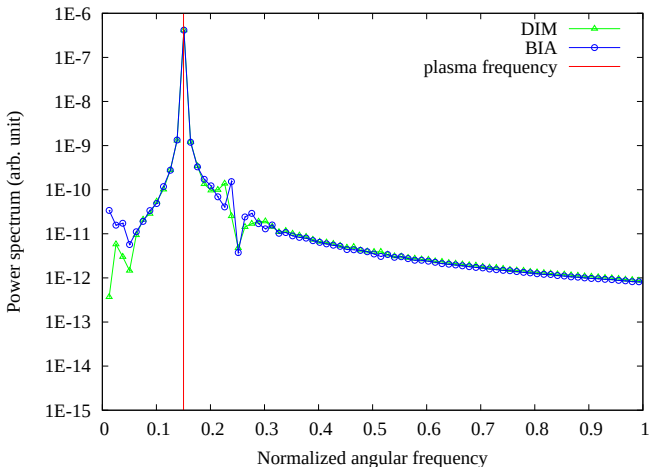


Figure 3: FFT analysis on a scalar potential at a distant point $r_{\text{distant}} \gg R$. A sharp spectrum peak is found at a normalized frequency of 0.1447, as indicated by a vertical line in red, which coincides with the normalized plasma frequency $\Pi$.

The original BIA scheme given in Eqs. (6) and (7) in such a case [10] is slightly modified as

$$m_i \Delta \boldsymbol{r}_i = m_i \Delta \boldsymbol{r}_{0,i} + \sum_{j \neq i}^{N} \mu_{ij} \left( \Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij} \Delta t \right), \tag{26}$$

$$m_i \Delta \boldsymbol{v}_i = m_i \Delta \boldsymbol{v}_{0,i} + \sum_{j \neq i}^{N} \mu_{ij} \Delta \boldsymbol{g}_{ij}, \tag{27}$$

where

$$\Delta \boldsymbol{r}_{0,i} = \boldsymbol{r}_i \left( \cos \Pi \Delta t - 1 \right) + \boldsymbol{v}_i \frac{\sin \Pi \Delta t}{\Pi}, \tag{28}$$

$$\Delta \boldsymbol{v}_{0,i} = \boldsymbol{r}_i \left( \cos \Pi \Delta t - 1 \right) + \boldsymbol{r}_i \Pi \sin \Pi \Delta t, \tag{29}$$

are the changes in position and velocity of $i$th electron due solely to $\boldsymbol{E}$, i.e. the background ions, during the time interval of $\Delta t$. Here $\Pi \equiv \sqrt{n_0 e^2 / 3 \varepsilon_0 m_e}$ is the plasma frequency in this case, where $m_e$ is the electron mass.

Figure 3 shows the FFT analysis on a potential $\varphi(\boldsymbol{r}_{\text{distant}})$ at a distant point $r_{\text{distant}} \gg R$ from the $N = 345$ system; one distributed ion and 344 electrons. A sharp peak at the normalized plasma frequency $\Pi = \sqrt{4\pi\epsilon_{\text{th}}/3m_e} = 0.1447$ is

found by using the BIA scheme as well as the DIM, where $\epsilon_{\rm th} = 2 \times 10^{-2}$ is the interaction parameter $U/K$ based on the average interparticle separation for $U$ and thermal speed for $K$.

### *3.3. Test Calculation III: Gravitational N-body problems*

We have applied the BIA scheme to gravitational $N$-body systems with initial conditions of $2K + U = 0$. The interparticle potential are modified using a Plummer radius $\delta$:

$$U_{ij}\left(r_{ij}\right) = -\frac{\mathcal{G}m_i m_j}{\sqrt{r_{ij}^2 + \delta^2}}. \tag{30}$$

Figure 4 for $N = 344$ compares the BIA with the 4th order Hermite integrator [11] in terms of the energy conservation, and the average errors in the individual position and velocity, i.e., the distances (standard deviations) $\sigma_r$ in $3N$-dimensional configuration space and $\sigma_v$ in $3N$-dimensional velocity space; both the standard deviations based on the 5th order RKF. For example

$$^{\rm BIA}\sigma_r \equiv \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(^{\rm BIA}\boldsymbol{r}_i - ^{\rm RKF}\boldsymbol{r}_i\right)^2} \tag{31}$$

defines the error in position for the BIA, since 5th order RKF is the most accurate scheme among the schemes used in this study.

As shown in Fig. 4, several errors for $N$=344 are depicted as a function of the time step size $\delta t \equiv 1/N_{\rm step}$, where $N_{\rm step}$ is the number of time-steps for a fixed time-interval of $1 \times \Delta t = n^{-1/3}/g_{\rm th}$. Both the BIA and 4th order Hermite (denoted by MHT4, homemade code) are serial (one thread) codes executed on a CPU. The relative energy errors are plotted in black, among which the RKF5 (a variable time-step scheme with $N_{\rm step} = 1,649$) is the best as expected. The energy error $\Delta E/E$ of the HMT4 showing the 4th order decrement with increasing $N_{\rm step}$ is much better in attainable error level of $10^{-14}$ at $N_{\rm step} \sim 10^4$ than the BIA showing the 2nd order decrement with the attainable error level of $10^{-10}$ also at $N_{\rm step} \sim 10^4$. However, as for the individual errors $\sigma_r$ and $\sigma_v$, the BIA showing 2nd order decrement is much better than the HMT4 with the 1st order decrement up to $N_{\rm step} = 10^6$. Such a 1st order decrement in individual errors was reported in Ref. [1]. Although $^{\rm HMT}\sigma$s are still decreasing linearly at $N_{\rm step} = 10^6$ the elapsed time has already reached around $10^4$ sec.

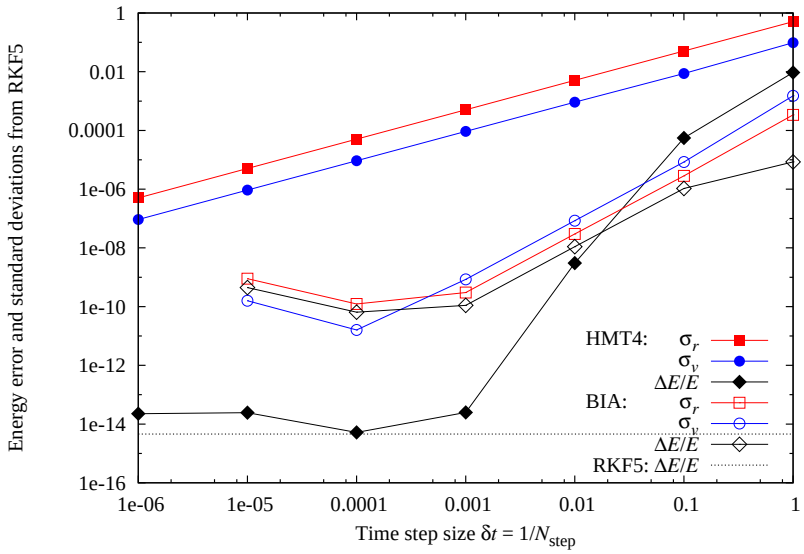


Figure 4: Comparison of the BIA with the 4th order Hermite integrator for $N = 344$ with initial condition of $2K + U = 0$, $\epsilon = -5.6 \times 10^{-3}$ and $\delta^2 = 10^{-4}$.

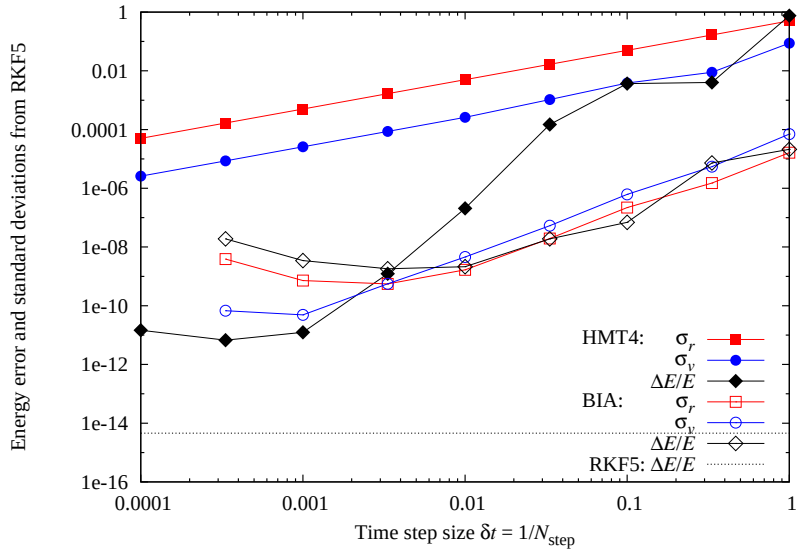


Figure 5: Comparison of the BIA with the 4th order Hermite integrator for $N = 9,262$ with initial condition of $2K + U = 0$, $\epsilon = -6.4 \times 10^{-4}$ and $\delta^2 = 10^{-4}$.

Similar error tendencies for $N = 9,262$ are shown in Fig. 5. In the cases for Figs. 4 and 5, the ratio of elapsed time of the BIA to that of the HMT4 is almost the same around 19 except for small $N_{\rm step} < 100$. Thus, if we could somehow improve the energy error of the BIA over the Hermite scheme with the same elapsed time without deteriorating $\sigma_r$ and $\sigma_v$, the BIA would be the better one than the 4th order Hermite scheme. For this purpose, we introduce an energy error correction scheme to the BIA, in which the energy error is corrected using the following position modification $\boldsymbol{r}_i \leftarrow \boldsymbol{r}'_i$ for $i = 1, 2, \ldots, N$:

$$\boldsymbol{r}'_i := \frac{\boldsymbol{r}_i}{1 - \dfrac{\Delta E}{U}}, \tag{32}$$

which leads to vanishing energy error $\Delta E'$, since

$$\Delta E' = \Delta K + \Delta U' = \Delta K + \Delta U - \Delta E = 0. \tag{33}$$

The top-left of Fig. 6 shows that the total wall-clock time of the BIA is set similar to that of the HMT for $N$=28. The energy error correction for BIA (denoted by cBIA in the figure) works, as shown in the top-right figure without deteriorating the individual errors in position (bottom-left) and in velocity (bottom-right). Changes, or strictly speaking errors, in $\sigma$s occur, however, they are to small to see in the figure. The energy error correction described in Eq. (32) is applied to the BIA occasionally when the normalized physical time $t$ is a multiple of $\Delta t$, i.e., $t = \Delta t, 2\Delta t, \ldots, 100 \times \Delta t$. Note that at around $N_{\rm step} \sim 30$, the energy errors for the RKF deteriorate abruptly. This is the result of a formation of what astrophysicists call the binary stars, in which two stars or particles are orbiting around with each other. After this time, the deviations, $\sigma$s, from the RKF cannot be regarded as the *errors* in respective $3N$-dimensional spaces.

## 4. Discussion and Conclusions

The error analysis of the binary interaction approximation (BIA) to the $N$-body problems was made to give the expressions for errors in the total angular momentum, and the total energy of the $N$-body system.

The BIA scheme is applied to two- and three-dimensional Coulombic and gravitational multibody systems. The BIA conserves total linear momenta in principle, and is a *pair-wise* variable time step scheme when used with the integrator using the embedded formula such as the Runge-Kutta-Fehlberg scheme. The total

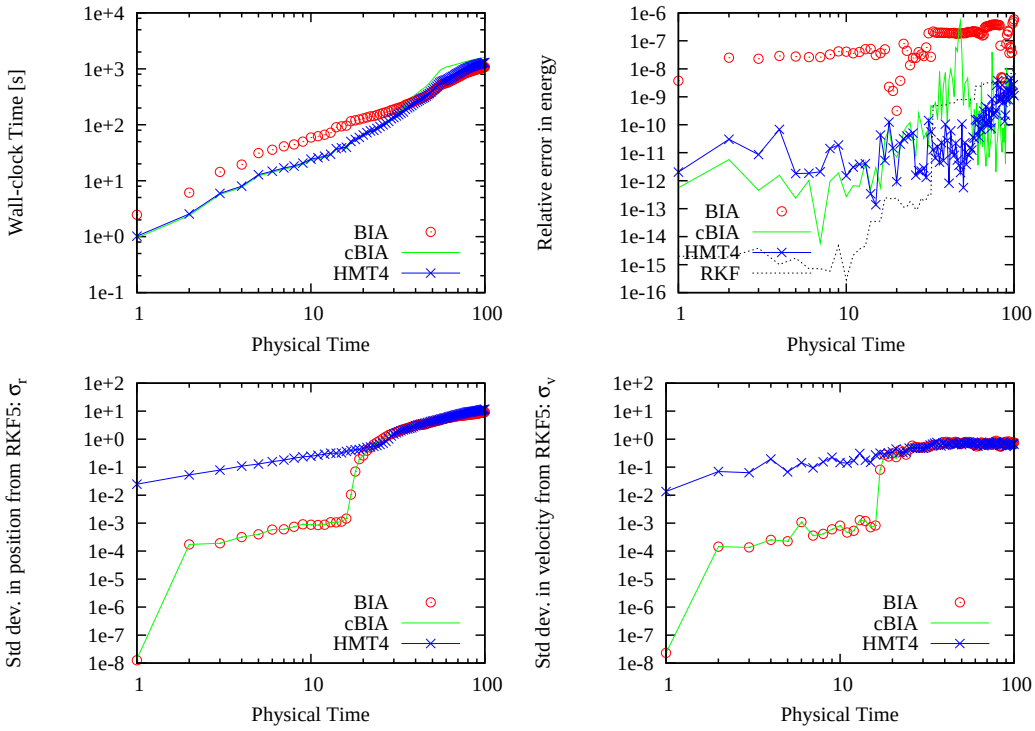


Figure 6: Energy error correction on BIA position for $N$=28, $2K + U = 0$, and $\delta^2 = 10^{-4}$. The elapsed times are similar among the BIA with and without energy correction and the HMT. Total physical system time calculated is $100 \times \Delta t$.

energy conservation is greatly improved by introducing the energy error correction scheme without deteriorating the individual errors in position and in velocity. The numerical results presented here are for low density and high temperature gas plasma, i.e. $\epsilon \ll 1$, which is the most appropriate for the BIA, as well as the gravitational $N$-body systems with $2K + U = 0$.

It should be noted that the BIA scheme is applicable to the tree method, the PPPM, in both of which distant particles from the particle under consideration are combined into one *super* particle or distributed potential source within a mesh (or a point source at a grid point), and neighboring particles are treated as they are. In the BIA such super particles and distributed potential sources are treated as particles to integrate Eq. (1) with replacing $N$ by $N_{\rm source} + N_{\rm neighbor}$.

Suppose a simple two-dimensional $N$-body problem, in which particles exist in a square region divided into $5 \times 5$ meshes, as shown in Fig. 7. The filled circle within the center mesh represents the particle-$i$ under force ($\boldsymbol{F}_i$) evaluation in the case of PPPM. The open circles in the same mesh and the 8 adjacent meshes represent other particle-$j$'s. In conventional PPPM schemes, the forces $\boldsymbol{F}_{ij}$ due to such neighboring particles are directly calculated and summed, and in the case of the PPPM-BIA the interaction ($\Delta\boldsymbol{r}_{ij}$ and $\Delta\boldsymbol{g}_{ij}$) are evaluated for a time interval of $\Delta t$. The rest of the particles in the system belong to the meshes in gray, and each mesh has its own mass or charge distribution $\rho_j(\boldsymbol{r})$, from which the remaining forces on particle-$i$ are evaluated and summed to give the total force $\boldsymbol{F}_i$ on particle-$i$ in the conventional PPPM, while $\Delta\boldsymbol{r}_{ij}$ and $\Delta\boldsymbol{g}_{ij}$ due to $\rho_j(\boldsymbol{r})$ are summed to give $\Delta\boldsymbol{r}_i$ and $\Delta\boldsymbol{v}_i$ in the PPPM-BIA.

In conclusion, given the particle positions in each mesh as in Fig. 7, the PPPM-BIA scheme is easily applied to the $N$-body system, by simply replacing the conventional time integrator used in the conventional PPPM, such as the RKF, the leap-frog and the Hermite scheme, etc., with the BIA scheme. Conventional integrators require summation of forces $\boldsymbol{F}_i = \sum_{j\neq i}^{N} \boldsymbol{F}_{ij}$ several times, depending on the integrator used, while the BIA requires the summation of the exact binary changes $\mu_{ij}\delta\boldsymbol{r}_{ij}$ and $\mu_{ij}\Delta\boldsymbol{g}_{ij}$ only once to give the increments $\Delta\boldsymbol{r}_i$ and $\Delta\boldsymbol{v}_i$.

It should also be noted that the calculation of changes $\mu_{ij}\delta\boldsymbol{r}_{ij}$ and $\mu_{ij}\Delta\boldsymbol{g}_{ij}$ can be done completely in parallel; the BIA analyses reported in Refs. [10], [12], and [13] used the general purpose graphics processing unit (GPGPU).

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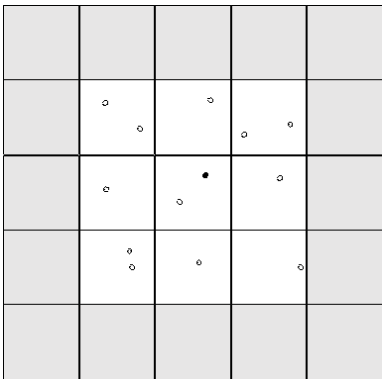

Figure 7: Application of the BIA to PPPM. The filled circle within the center mesh represents the particle-*i* under force evaluation in the case of PPPM. The open circles in the same mesh and the 8 adjacent meshes represent other particle-*j*'s. The rest of the particles in the system belong to the meshes in gray.

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## References

[1] T. Boekholt, S. P. Zwart, On the reliability of *N*-body simulations, Computational Astrophysics and Cosmology 2015, 2:2 (2015) 1–21.

[2] D. Sugimoto, Y. Chikada, J. Makino, T. Ito, T. Ebisuzaki, M. Umemura, A Special-purpose computer for gravitational many-body problems, Nature 345 (3) (1990) 33–35.

[3] J. Makino, M. Taiji, T. Ebisuzaki, D. Sugimoto, GRAPE-4: A Massively Parallel Special-Purpose Computer for Collisional *N*-Body Simulations, APJ 480 (1997) 432–446.

[4] A. W. Appel, An Efficient Program for Many-Body Simulation, SIAM J. Sci. Stat. Comput. 6 (1985) 85–103.

[5] J. E. Barnes, P. Hutt, A hierarchical O($N$log$N$) force-calculation algorithm, Nature 324 (1986) 446–449.

[6] P. P. Brieu, F. J. Summers, J. P. Ostriker, Cosmological Simulations Using Special Purpose Computers: Implementing $P^3M$ on GRAPE, APJ 453 (1995) 566.

[7] S. Oikawa, H. Funasaka, Binary Interaction Approximation to *N*-Body Problems, Plasma Fusion Res. 5 (2010) S1051.

[8] E. Fehlberg, Low-order classical Runge-Kutta formulas with step size control and their application to some heat transfer problems, Nasa technical report, NASA-TR-R-315 (1969).

[9] E. Fehlberg, Klassische Runge-Kutta-Formeln vierter und niedrigerer Ordnung mit Schrittweiten-Kontrolle und ihre Anwendung auf Warmeleitungsprobleme, Computing (Arch. Elektron. Rechnen) 6 (1970) 61–71.

[10] S. Oikawa, T. Kamei, and M. Goto, Application of the Binary Interaction Approximation to Plasma Oscillation, Plasma Fusion Res. 7 (2012) 2401101.

[11] J. Makino, Optimal order and time-step criterion for Aarseth-type N-body integrators, APJ 369 (3) (1991) 200–212.

[12] S. Oikawa, M. Goto, K. Haruta, and T. Kamei, Accuracy Assurance in Binary Interaction Approximation for *N*-body Problems, Plasma Fusion Res. 7 (2012) 2401103.

[13] S. Oikawa and T. Kamei, Accuracy Assurance in Binary Interaction Approximation for *N*-body Problems II, Plasma Fusion Res. 8 (2013) 2401091.

## Appendix A. Derivation of Errors $L$ and $E$ in BIA scheme

*Appendix A.1.* $\Delta \boldsymbol{L}$ *in BIA*

The change in the angular momentum, $\Delta \boldsymbol{L}$, calculated by using the BIA scheme is given as

$$\begin{aligned} \Delta \boldsymbol{L} &= \sum_{i=1}^{N} \Big[ (\boldsymbol{r}_i + \boldsymbol{v}_i \Delta t + \delta \boldsymbol{r}_i) \times \Delta \boldsymbol{p}_i + (\boldsymbol{v}_i \Delta t + \delta \boldsymbol{r}_i) \times \boldsymbol{p}_i \Big] \\ &= \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left[ (\boldsymbol{r}_i + \boldsymbol{v}_i \Delta t + \delta \boldsymbol{r}_i) \times \Delta \boldsymbol{p}_{ij} + \frac{\mu_{ij}}{m_i} \left( \Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij} \Delta t \right) \times \boldsymbol{p}_i \right], \quad \text{(A.1)} \end{aligned}$$

where $m_i\delta\boldsymbol{r}_i = \sum_{j\neq 1}^{N}\mu_{ij}\left(\Delta\boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t\right) \equiv \sum_{j\neq 1}^{N}\mu_{ij}\delta\boldsymbol{r}_{ij}$ has been used, as was shown in Fig. 2. Substituting $m_i\boldsymbol{r}_i = m_i\boldsymbol{R}_{ij} + \mu_{ij}\boldsymbol{r}_{ij}$ and $\boldsymbol{p}_i = m_i\boldsymbol{v}_i = m_i\boldsymbol{G}_{ij} + \mu_{ij}\boldsymbol{g}_{ij}$, we have

$$\begin{aligned}
\Delta\boldsymbol{L} &= \sum_{i=1}^{N}\sum_{j\neq i}^{N}\left[\left(\boldsymbol{R}_{ij} + \boldsymbol{G}_{ij}\Delta t\right)\times\Delta\boldsymbol{p}_{ij} + \mu_{ij}\left(\Delta\boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t\right)\times\boldsymbol{G}_{ij}\right] \\
&+ \sum_{i=1}^{N}\sum_{j\neq i}^{N}\left\{\left[\frac{\mu_{ij}}{m_i}\left(\boldsymbol{r}_{ij} + \boldsymbol{g}_{ij}\Delta t\right) + \delta\boldsymbol{r}_i\right]\times\Delta\boldsymbol{p}_{ij} + \frac{\mu_{ij}}{m_i}\Delta\boldsymbol{r}_{ij}\times\boldsymbol{p}_{ij}\right\} \\
&\equiv \Delta\boldsymbol{L}^{RG} + \Delta\boldsymbol{L}^{rg}, \qquad \text{(A.2)}
\end{aligned}$$

where the first term $\Delta\boldsymbol{L}^{RG}$ includes *individual* center of mass quantities of $\boldsymbol{R}_{ij}$ and $\boldsymbol{G}_{ij}$, and the second term $\Delta\boldsymbol{L}^{rg}$ does not.

$$\begin{aligned}
\Delta\boldsymbol{L}^{RG} &= \sum_{i=1}^{N}\sum_{j\neq i}^{N}\left(\boldsymbol{R}_{ij} + \boldsymbol{G}_{ij}\Delta t\right)\times\Delta\boldsymbol{p}_{ij} + \sum_{i=1}^{N}\sum_{j\neq i}^{N}\mu_{ij}\delta\boldsymbol{r}_{ij}\times\boldsymbol{G}_{ij} \\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[\left(\boldsymbol{R}_{ij} + \boldsymbol{G}_{ij}\Delta t\right)\times\Delta\boldsymbol{p}_{ij} + \left(\boldsymbol{R}_{ji} + \boldsymbol{G}_{ji}\Delta t\right)\times\Delta\boldsymbol{p}_{ji}\right] \\
&+ \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\mu_{ij}\delta\boldsymbol{r}_{ij}\times\boldsymbol{G}_{ij} + \mu_{ji}\delta\boldsymbol{r}_{ji}\times\boldsymbol{G}_{ji}\right) \\
&= 0, \qquad \text{(A.3)}
\end{aligned}$$

since $\boldsymbol{R}_{ji} = \boldsymbol{R}_{ij}, \boldsymbol{G}_{ji} = \boldsymbol{G}_{ij}$ and $\Delta\boldsymbol{p}_{ij} + \Delta\boldsymbol{p}_{ji} = 0$. Similarly, the remaining term, $\Delta\boldsymbol{L}^{rg}$, is

$$\begin{aligned}
\Delta\boldsymbol{L}^{rg} &= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left\{\delta\boldsymbol{r}_i - \delta\boldsymbol{r}_j + \left[\frac{\mu_{ij}}{m_i}\left(\boldsymbol{r}_{ij} + \boldsymbol{g}_{ij}\Delta t\right) - \frac{\mu_{ji}}{m_j}\left(\boldsymbol{r}_{ji} + \boldsymbol{g}_{ji}\Delta t\right)\right]\right\}\times\Delta\boldsymbol{p}_{ij} \\
&+ \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\frac{\mu_{ij}}{m_i}\Delta\boldsymbol{r}_{ij} - \frac{\mu_{ji}}{m_j}\Delta\boldsymbol{r}_{ji}\right)\times\boldsymbol{p}_{ij} \\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[\delta\boldsymbol{r}_i - \delta\boldsymbol{r}_j + \left(\frac{1}{m_i} + \frac{1}{m_j}\right)\mu_{ij}\left(\boldsymbol{r}_{ij} + \boldsymbol{g}_{ij}\Delta t\right)\right]\times\Delta\boldsymbol{p}_{ij} \\
&+ \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\frac{1}{m_i} + \frac{1}{m_j}\right)\mu_{ij}\Delta\boldsymbol{r}_{ij}\times\boldsymbol{p}_{ij} \\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left\{\left(\delta\boldsymbol{r}_i - \delta\boldsymbol{r}_j\right)\times\Delta\boldsymbol{p}_{ij} + \left(\boldsymbol{r}_{ij} + \boldsymbol{g}_{ij}\Delta t\right)\times\Delta\boldsymbol{p}_{ij} + \Delta\boldsymbol{r}_{ij}\times\boldsymbol{p}_{ij}\right\}, \qquad \text{(A.4)}
\end{aligned}$$

where use was made of $m_i^{-1} + m_j^{-1} = \mu_{ij}^{-1}$. Since the BIA scheme gives angular momentum conservation for each binary system, i.e., $\Delta \boldsymbol{L}_{ij} = \left(\boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_{ij}\right) \times \Delta \boldsymbol{p}_{ij} + \Delta \boldsymbol{r}_{ij} \times \boldsymbol{p}_{ij} = 0$, we have finally the error in the total angular momentum by using the BIA scheme given in Eq. (18).

$$\Delta \boldsymbol{L} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[\left(\delta \boldsymbol{r}_i - \delta \boldsymbol{r}_j\right) - \delta \boldsymbol{r}_{ij}\right] \times \Delta \boldsymbol{p}_{ij}.$$

*Appendix A.2. $\Delta E$ in BIA*

The total energy is given by:

$$E = K + U = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} U_{ij}. \tag{A.5}$$

Noting that $\boldsymbol{r}_{ij}(\Delta t) = \boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_i - \Delta \boldsymbol{r}_j$, we have

$$\Delta K = \sum_{i=1}^{N} \left(\boldsymbol{v}_i + \frac{1}{2}\Delta \boldsymbol{v}_i\right) \cdot \Delta \boldsymbol{p}_i, \tag{A.6}$$

$$\Delta U = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[U_{ij}\left(\boldsymbol{r}_{ij} + \Delta \boldsymbol{r}_i - \Delta \boldsymbol{r}_j\right) - U_{ij}\left(\boldsymbol{r}_{ij}\right)\right]. \tag{A.7}$$

The change in the total energy $\Delta K$ is

$$\begin{aligned} \Delta K &= \sum_{i=1}^{N} \boldsymbol{v}_i \cdot \sum_{j \neq i}^{N} \Delta \boldsymbol{p}_{ij} + \frac{1}{2} \sum_{i=1}^{N} \frac{1}{m_i} \sum_{k \neq i}^{N} \Delta \boldsymbol{p}_{ik} \cdot \sum_{j \neq i}^{N} \Delta \boldsymbol{p}_{ij} \\ &= \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left(\boldsymbol{G}_{ij} + \frac{\boldsymbol{p}_{ij}}{m_i}\right) \cdot \Delta \boldsymbol{p}_{ij} + \frac{1}{2} \sum_{i=1}^{N} \frac{1}{m_i} \sum_{j \neq i}^{N} \Delta \boldsymbol{p}_{ij} \cdot \sum_{k \neq i}^{N} \Delta \boldsymbol{p}_{ik} \\ &\equiv \Delta K^G + \Delta K^g, \end{aligned} \tag{A.8}$$

where the first term including the mass velocity $\boldsymbol{G}_{ij}$ for the pair $ij$ is

$$\begin{aligned} \Delta K^G &= \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left(\boldsymbol{G}_{ij} \cdot \Delta \boldsymbol{p}_{ij} + \boldsymbol{G}_{ji} \cdot \Delta \boldsymbol{p}_{ji}\right) \\ &= \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \boldsymbol{G}_{ij} \cdot \left(\Delta \boldsymbol{p}_{ij} + \Delta \boldsymbol{p}_{ji}\right) \\ &= 0, \end{aligned} \tag{A.9}$$

312 whereas the second term not including $\boldsymbol{G}_{ij}$ is

$$\begin{aligned}
\Delta K^g &= \sum_{i=1}^{N}\sum_{j\neq i}^{N}\frac{\boldsymbol{p}_{ij}}{m_i}\cdot\Delta\boldsymbol{p}_{ij}+\frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}\sum_{j\neq i}^{N}\Delta\boldsymbol{p}_{ij}\cdot\sum_{k\neq i}^{N}\Delta\boldsymbol{p}_{ik}\\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\frac{1}{m_i}+\frac{1}{m_j}\right)\boldsymbol{p}_{ij}\cdot\Delta\boldsymbol{p}_{ij}+\frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}\sum_{j\neq i}^{N}\left(\Delta\boldsymbol{p}_{ij}+\sum_{k\neq i,j}^{N}\Delta\boldsymbol{p}_{ik}\right)\cdot\Delta\boldsymbol{p}_{ij}\\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\frac{1}{m_i}+\frac{1}{m_j}\right)\left(\boldsymbol{p}_{ij}+\frac{1}{2}\Delta\boldsymbol{p}_{ij}\right)\cdot\Delta\boldsymbol{p}_{ij}\\
&+ \frac{1}{2}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\frac{1}{m_i}\sum_{k\neq i,j}^{N}\Delta\boldsymbol{p}_{ik}-\frac{1}{m_j}\sum_{k\neq i,j}^{N}\Delta\boldsymbol{p}_{jk}\right)\cdot\Delta\boldsymbol{p}_{ij}\\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\boldsymbol{g}_{ij}+\frac{1}{2}\Delta\boldsymbol{g}_{ij}\right)\cdot\Delta\boldsymbol{p}_{ij}\\
&+ \frac{1}{2}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[\left(\Delta\boldsymbol{g}_i-\Delta\boldsymbol{g}_j\right)-\Delta\boldsymbol{g}_{jj}\right]\cdot\Delta\boldsymbol{p}_{ij}. \qquad \text{(A.10)}
\end{aligned}$$

313 Note that

$$\begin{aligned}
\Delta E_{ij} &= \Delta K_{ij}+\Delta U_{ij}\\
&= \left(\boldsymbol{g}_{ij}+\frac{1}{2}\Delta\boldsymbol{g}_{ij}\right)\cdot\Delta\boldsymbol{p}_{ij}+U_{ij}\left(\boldsymbol{r}_{ij}+\Delta\boldsymbol{r}_{ij}\right)-U_{ij}\left(\boldsymbol{r}_{ij}\right)\\
&= 0, \qquad \text{(A.11)}
\end{aligned}$$

314 from which

$$\begin{aligned}
\Delta E &= \Delta K+\Delta U\\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\boldsymbol{g}_{ij}+\frac{1}{2}\Delta\boldsymbol{g}_{ij}\right)\cdot\Delta\boldsymbol{p}_{ij}+\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[\left(\Delta\boldsymbol{g}_i-\Delta\boldsymbol{g}_j\right)-\Delta\boldsymbol{g}_{ij}\right]\cdot\Delta\boldsymbol{p}_{ij}\\
&+ \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[U_{ij}\left(\boldsymbol{r}_{ij}+\Delta\boldsymbol{r}_{ij}+\delta\hat{\boldsymbol{r}}_{ij}\right)-U_{ij}\left(\boldsymbol{r}_{ij}\right)\right]\\
&= \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[U_{ij}\left(\boldsymbol{r}_{ij}\right)-U_{ij}\left(\boldsymbol{r}_{ij}+\Delta\boldsymbol{r}_{ij}\right)\right]+\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left[\left(\Delta\boldsymbol{g}_i-\Delta\boldsymbol{g}_j\right)-\Delta\boldsymbol{g}_{ij}\right]\cdot\Delta\boldsymbol{p}_{ij}
\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[ U_{ij}\left( \boldsymbol{r}_{ij} + \Delta\boldsymbol{r}_{ij} + \delta\hat{\boldsymbol{r}}_{ij} \right) - U_{ij}\left( \boldsymbol{r}_{ij} \right) \right] \\
&= \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[ \left( \Delta\boldsymbol{g}_i - \Delta\boldsymbol{g}_j \right) - \Delta\boldsymbol{g}_{ij} \right] \cdot \Delta\boldsymbol{p}_{ij} \\
&+ \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[ U_{ij}\left( \boldsymbol{r}_{ij} + \Delta\boldsymbol{r}_{ij} + \delta\hat{\boldsymbol{r}}_{ij} \right) - U_{ij}\left( \boldsymbol{r}_{ij} + \Delta\boldsymbol{r}_{ij} \right) \right]. \qquad \text{(A.12)}
\end{aligned}
$$

315 Thus, we have the errors in the total angular momentum and the total energy:

$$
\Delta\boldsymbol{L} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \delta\hat{\boldsymbol{r}}_{ij} \times \Delta\boldsymbol{p}_{ij}, \qquad \text{(A.13)}
$$

$$
\Delta E = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left( \delta\hat{\boldsymbol{g}}_{ij} \cdot \Delta\boldsymbol{p}_{ij} + \delta\hat{U}_{ij} \right), \qquad \text{(A.14)}
$$

316 where

$$
\delta\hat{U}_{ij} \equiv U\left( \boldsymbol{r}_{ij} + \Delta\boldsymbol{r}_{ij} + \delta\hat{\boldsymbol{r}}_{ij} \right) - U\left( \boldsymbol{r}_{ij} + \Delta\boldsymbol{r}_{ij} \right). \qquad \text{(A.15)}
$$