Application of the Binary Interaction Approximation to Plasma Oscillation*)

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The BIA (Binary Interaction Approximation) formulation in the presence of neutralizing immovable background ion is presented for analysis of multiple electron motion. Such a BIA scheme is applied to electrons in plasmas. A test calculation shows that 1) the plasma oscillation and its frequency are successfully detected, 2) the CPU time for the BIA are less than 1.5 sec and 1 hour for two and three dimensional analysis, while 127 sec and 13 hours for the direct integration method (DIM) by using a Runge-Kutta-Fehlberg integrator with an absolute error tolerance of 10^{-16}, and 3) the number of time steps for the DIM, in such a case, are as many as 5.8×10^4 and 3.6×10^6, while those for the BIA are only 256 and 512.

Keywords: N-body problem, binary interaction approximation, plasma oscillation, background ion, Fourier analysis

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1. Introduction

We have proposed the Binary Interaction Approximation (BIA) scheme [1–3] to N-body problems. The BIA scheme views an N-body problem as the superposition of ${}_NC_2$ two-body problems [1]. One of the most fundamental phenomena occurring in plasmas is the plasma oscillation. Equation of motion is given as

$$m_i \frac{\mathrm{d}\boldsymbol{v}_i}{\mathrm{d}t} = \frac{Z_i e^2}{4\pi\varepsilon_0} \sum_{j\neq i}^{N} Z_j \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|^3}. \tag{1}$$

For $N \gg 1$, it is practically impossible for the large number of particles, 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 tends to increase with increasing number of particles N, so the total CPU time should scale as $N^{2.3-3}$.

The efficient, 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]. 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 [7].

2. Original BIA Scheme

Let us give a brief review on the original BIA scheme proposed by the authors [1]. First choose a particle pair (i, j) from N particles as shown in Fig. 1. There are ${}_NC_2 = N(N+1)/2$ combinations. The equation of motion for this case is:

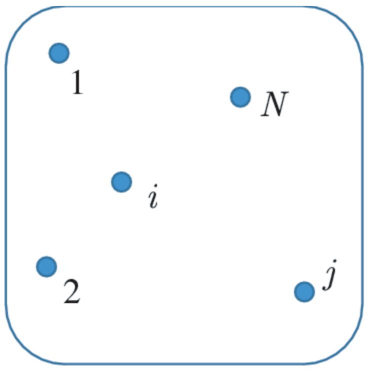

Fig. 1 An N-body system.

$$\mu_{ij} \frac{\mathrm{d}\boldsymbol{g}_{ij}}{\mathrm{d}t} = \frac{Z_i Z_j e^2}{4\pi\varepsilon_0} \frac{\boldsymbol{r}_{ij}}{r_{ij}^3}, \tag{2}$$

where $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $\boldsymbol{g}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$, and μ_{ij} is the reduce mass.

Since the exact solution to two-body problem is known, for any time interval Δt the solution, $\boldsymbol{r}_{ij}(\Delta t)$ and $\boldsymbol{g}_{ij}(\Delta t)$ are easily found from the initial conditions of $\boldsymbol{r}_{ij}(0)$ and $\boldsymbol{g}_{ij}(0)$. Once the solutions to all the two-body systems have been found, changes in position and velocity of individual particle during given time interval Δt is calculated as follows:

$$m_i \Delta\boldsymbol{r}_i = m_i \boldsymbol{v}_i \Delta t + \sum_{j\neq i}^{N} \mu_{ij} \left(\Delta\boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t\right), \tag{3}$$

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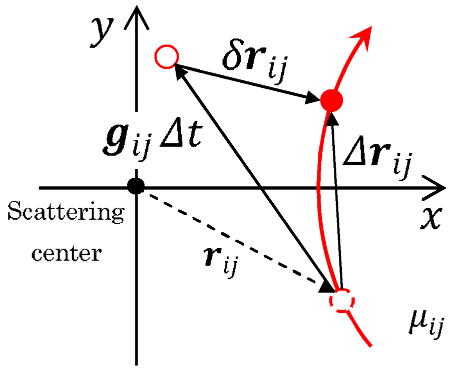

Fig. 2 Relative motion for particle pair (i, j). Scattering center is at the origin. The change in position of the particle with a mass μ_{ij} is $\Delta \boldsymbol{r}_{ij}$. If no interaction occurs, the change in position is $\boldsymbol{g}_{ij}\Delta t$ during a time interval of Δt.

$$m_i \Delta \boldsymbol{v}_i = \sum_{j\neq i}^{N} \mu_{ij} \Delta \boldsymbol{g}_{ij}. \tag{4}$$

Equation (4) for the velocity, i.e. momentum changes ensures the momentum conservation of the entire system. It should be noted that, unlike the changes in velocity $\Delta \boldsymbol{v}_i$, changes in position $\Delta \boldsymbol{r}_i$ due to particle j is not simple summation over $\Delta \boldsymbol{r}_{ij}$. As shown in, and explained in the caption of Fig. 2, the subtraction by $\boldsymbol{g}_{ij}\Delta t$ from total change in position $\Delta \boldsymbol{r}_{ij}$ gives change in position due solely to the interaction between the pair (i, j). In the limit $\Delta t \to 0$, Eq. (3) reduces to the definition of velocity, and Eq. (4) reduces to the original equation of motion, as given in Eq. (1).

3. BIA Formulation for Electrons in the Presence of Background Ions

Suppose N electrons are in the presence of uniformly distributed immovable background ions. In such a case, the electric field and the electrostatic potential due to the ions are given by

$$\boldsymbol{E}(r) = \frac{n_0 e \boldsymbol{r}}{3\varepsilon_0}, \ \varphi(r) = -\frac{n_0 e r^2}{6\varepsilon_0}, \tag{5}$$

where n_0 stands for the ion number density. Thus the equation of motion for i-th electron is as follows:

$$m_i \frac{\mathrm{d}\boldsymbol{v}_i}{\mathrm{d}t} = -\frac{n_0 e^2}{3\varepsilon_0}\boldsymbol{r}_i + \frac{e^2}{4\pi\varepsilon_0}\sum_{j\neq i}^{N}\frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|^3}. \tag{6}$$

In this case, let us regard the background ions as the zero-th particle with infinite mass, then the relative system between i-th electron and the bulk of the background ions becomes

$$\frac{\mathrm{d}^2\boldsymbol{r}_i}{\mathrm{d}t^2} + \frac{n_0 e^2}{3 m_i \varepsilon_0}\boldsymbol{r}_i = 0, \tag{7}$$

since $\mu_{i0} =\equiv m_i \times \infty/(m_i + \infty) = m_i$ and $\boldsymbol{g}_{i0} = \boldsymbol{v}_i - 0 = \boldsymbol{v}_i$. Thus, the original BIA scheme, given in Eqs. (3) and (4), becomes as

$$m_i \Delta \boldsymbol{r}_i = m_i \Delta \boldsymbol{r}_{i0} + \sum_{\substack{j=1\\ j\neq i}}^{N} \mu_{ij}\left(\Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}\Delta t\right), \tag{8}$$

$$m_i \Delta \boldsymbol{v}_i = m_i \Delta \boldsymbol{g}_{i0} + \sum_{\substack{j=1\\ j\neq i}}^{N} \mu_{ij} \Delta \boldsymbol{g}_{ij}. \tag{9}$$

The first terms, both in Eq. (8) and Eq. (9), represent the respective changes due to plasma oscillation with an electron plasma frequency $\Pi \equiv \sqrt{n_0 e^2 / 3\varepsilon_0 m_e}$ given by

$$\Delta \boldsymbol{r}_i = \boldsymbol{r}_i (\cos \Pi\Delta t - 1) + \boldsymbol{v}_i \frac{\sin \Pi\Delta t}{\Pi},$$
$$\Delta \boldsymbol{v}_i = \boldsymbol{v}_i (\cos \Pi\Delta t - 1) - \boldsymbol{r}_i \Pi \sin \Pi\Delta t,$$

during a time interval of Δt.

4. Test Calculation

In this test calculation section, we will adopt the normalization system, as in Ref. [1], where lengths are normalized by an average interparticle separation $\Delta\ell = n_0^{-1/3}$, and velocities by a relative thermal speed between electrons, i.e. $g_{\mathrm{th}}^{ee} = \sqrt{2T/\mu_{ee}} = \sqrt{2}v_{\mathrm{th}}^{e}$.

4.1 Two dimensional analysis

Two-dimensional analysis is made with the BIA scheme for the number of particles is 122, 121 of which are electrons. An immovable background ion is centered at the origin; the initial electron distribution is uniform in the phase space $(\boldsymbol{r}, \boldsymbol{v})$.

The trajectories, in configuration and velocity spaces, of an electron are shown in Figs. 3 and 4, in which blue points are obtained by the BIA scheme, while a red line by the DIM (RKF65). Note that, in Fig. 4, there are several DIM line segments in red, on which only one or two BIA points are depicted. Since the time interval for adjacent BIA points is constant, the electron under consideration feels a strong force, i.e. the impulse, due to other electrons along the line segments.

The CPU time for the BIA in this calculation is less than 1.5 sec, while 127 sec for the DIM by using a Runge-Kutta-Fehlberg integrator [8] with an absolute error tolerance of 10^{-16}. It should be noted that the number of time steps for the DIM, in this case, is as many as 1.1 millions, while that for the BIA is only 256. In spite of much smaller number of time steps, as typically shown in Fig. 4, the complicated change in velocity with time, or the acceleration, is typically reproduced well with the BIA scheme.

Figure 5 depicts the time evolution of energy of the system: kinetic energy K in red, potential energy U in green, and the total energy $E = K + U$ in blue of the entire system. This figure shows the energy conservation, $E = K + U = \mathrm{const}$, and the normalized period for energy K and U is around 280.0, twice of which gives the 560.0. The corresponding theoretical plasma oscillation in this case is

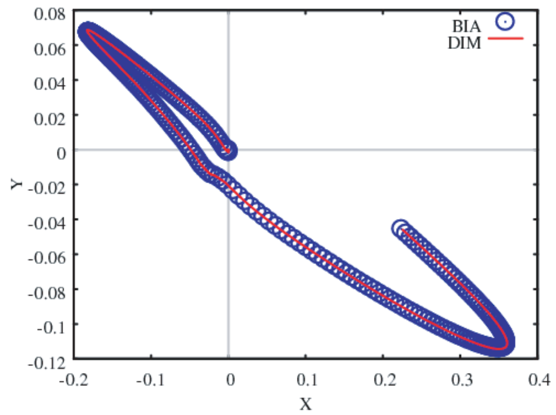

Fig. 3 Two-dimensional electron trajectory initially at rest in the configuration space for a 122-body system. A red line represents that by using the direct integration method: DIM. Blue circles indicate the trajectory obtained by using the BIA scheme.

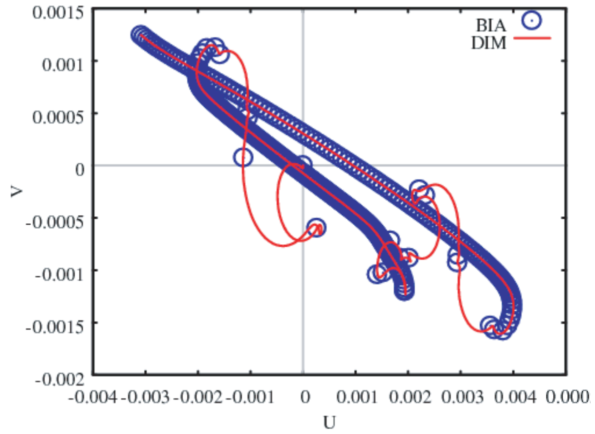

Fig. 4 Two-dimensional electron trajectory in the velocity space for a 122-body system. A red line represents that by using the direct integration method: DIM. Blue circles indicate the trajectory obtained by using the BIA scheme.

$$T = 2\pi/\Pi = 560.5, \tag{10}$$

which is close to that obtained by using the BIA analysis.

4.2 Three dimensional analysis

Similar calculation in three dimensions is made for the number of particles is 344, 343 of which are electrons. An immovable neutralizing positive *point* charge (ion), in this case, is at the origin. The electrons are randomly distributed around the positive charge initially with an average interparticle separation $\Delta\ell = n_0^{-1/3}$ and velocity distribution is also uniform around their thermal speed.

Figure 6 depicts the time evolution of x-coordinate of an electron, in which green points are obtained by the BIA scheme, while a red line by the DIM, i.e. RKF65. The position of the electron by using the BIA begins to deviate from that by the DIM after around the normalized time of 3.8, until then the agreement is excellent.

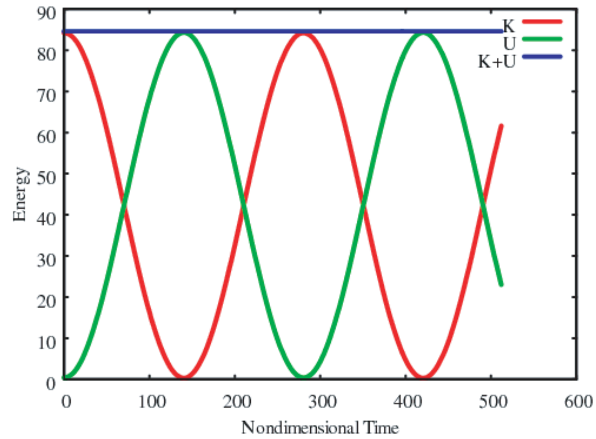

Fig. 5 Time dependent energy for a two N-body system, calculated by using the BIA scheme. K and U stand for the kinetic and potential energy of the system, respectively.

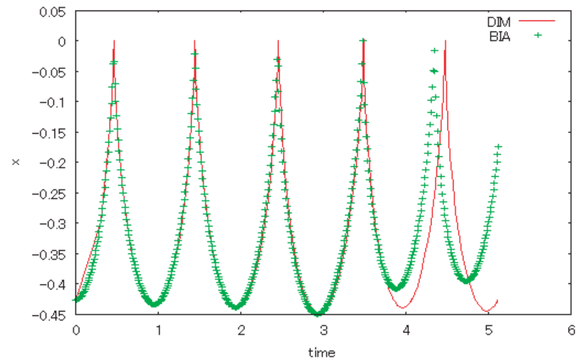

Fig. 6 Comparison of the time-dependent x-coordinate of an electron in the configuration space for a 344-body system in three-dimensions. A red line represents that by using the direct integration method: DIM. Green points indicate that obtained by using the BIA scheme.

Using FFT analysis on the electrostatic potential $\varphi(\boldsymbol{r}_0)$ at a point $\boldsymbol{r}_0$, a spectrum peak is found at a normalized period of 1.28, which is close to the period for the normalized plasma frequency of 1.35, as marked with a red square in Fig. 7. It should be noted that, these calculations take the CPU time of 13 hours for the DIM and only 1 hour for the BIA.

5. Summary

The BIA (Binary Interaction Approximation) formulation, in the presence of neutralizing immovable background ion, is presented for analysis of multiple electron motion. Such a BIA scheme is applied to electrons in plasmas. The plasma oscillation and its frequency are successfully detected with much less CPU time than a conventional method, i.e. a Runge-Kutta-Fehlberg method with an absolute error tolerance of 10^{-16}.

Test calculations show, for two- and three-dimensional cases, that 1) the normalized period of

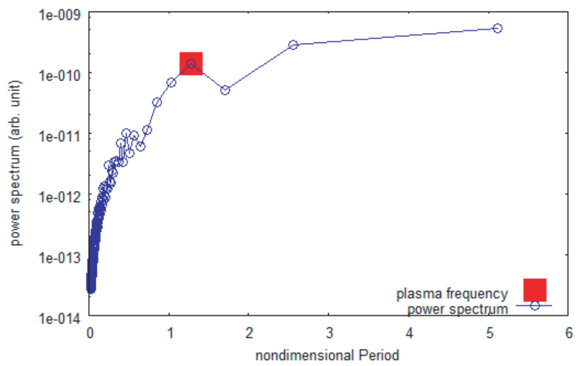

Fig. 7 FFT analysis on a scalar potential $\varphi(\boldsymbol{r}_0)$ at a point $\boldsymbol{r}_0$ for the same case shown in Fig. 5. A spectrum peak is found at a normalized frequency 1.28, as indicated by red square, close to the normalized plasma frequency of 1.35 as marked with a red square.

the plasma oscillation for two-/three-dimensional cases are successfully detected to be 560.0/1.28 when its theoretical value is 560.5/1.31, 2) test calculations for two/three dimensional case show that the CPU time for the BIA is less than 1.5 sec/1 hour, while 127 sec/13 hours for the DIM by using a Runge-Kutta-Fehlberg integrator with an absolute error tolerance of 10^{-16}, and 3) the number of time steps for the DIM, in such a case, is as many as around $5.8 \times 10^4/3.6 \times 10^6$, while that for the BIA is only 256/512.

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Appendix A. Derivation of BIA Scheme

Since the force terms in Eq. (1) are the summation of those in Eq. (2), we have

$$\boldsymbol{f}_i = \sum_{j\neq i}^{N} \boldsymbol{f}_{ij}\left(\boldsymbol{r}_i, \boldsymbol{r}_j\right). \tag{A.1}$$

The exact change $m_i \Delta \boldsymbol{v}_i$ in momentum of the particle-i during a time-interval Δt is formally given as

$$\begin{aligned} m_i \Delta \boldsymbol{v}_i &= \int_t^{t+\Delta t} \boldsymbol{f}_i\left(\boldsymbol{r}_i(t), \boldsymbol{r}_j(t)\right) \mathrm{d}t \\ &= \sum_{j\neq i}^{N} \int_t^{t+\Delta t} \boldsymbol{f}_{ij}\left(\boldsymbol{r}_i(t), \boldsymbol{r}_j(t)\right) \mathrm{d}t. \end{aligned} \tag{A.2}$$

Since, in the framework of the BIA via Eq. (2), the relative force $\boldsymbol{f}_{ij}(t)$ changes the relative momentum $\mu_{ij}\boldsymbol{g}_{ij}(t)$,

$$m_i \Delta \boldsymbol{v}_i \cong \sum_{j\neq i}^{N} \mu_{ij}\left[\boldsymbol{g}_{ij}(t+\Delta t) - \boldsymbol{g}_{ij}(t)\right] = \sum_{j\neq i}^{N} \mu_{ij}\Delta \boldsymbol{g}_{ij}, \tag{A.3}$$

which is Eq. (4).

Similarly, the exact change $\Delta \boldsymbol{r}_i$ in position of the particle-i during Δt is formally given by

$$\begin{aligned} \Delta \boldsymbol{r}_i &= \int_t^{t+\Delta t} \boldsymbol{v}_i(t')\,\mathrm{d}t' = \int_t^{t+\Delta t} \left[\boldsymbol{v}_i(t) + \Delta \boldsymbol{v}_i(t')\right] \mathrm{d}t' \\ &= \boldsymbol{v}_i(t)\,\Delta t + \int_t^{t+\Delta t} \mathrm{d}t' \int_t^{t'} \frac{\mathrm{d}\boldsymbol{v}_i(t'')}{\mathrm{d}t''} \mathrm{d}t'', \end{aligned} \tag{A.4}$$

from which, with the BIA scheme, we have

$$\begin{aligned} m_i \Delta \boldsymbol{r}_i &\cong m_i \boldsymbol{v}_i(t)\,\Delta t + \int_t^{t+\Delta t} \mathrm{d}t' \int_t^{t'} \sum_{j\neq i}^{N} \mu_{ij} \frac{\mathrm{d}\boldsymbol{g}_{ij}(t'')}{\mathrm{d}t''} \mathrm{d}t'' \\ &= m_i \boldsymbol{v}_i(t)\,\Delta t + \int_t^{t+\Delta t} \mathrm{d}t' \sum_{j\neq i}^{N} \mu_{ij}\left[\boldsymbol{g}_{ij}(t') - \boldsymbol{g}_{ij}(t)\right] \\ &= m_i \boldsymbol{v}_i(t)\,\Delta t + \sum_{j\neq i}^{N} \mu_{ij}\left[\Delta \boldsymbol{r}_{ij} - \boldsymbol{g}_{ij}(t)\,\Delta t\right], \end{aligned} \tag{A.5}$$

which is Eq. (3).

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