

# Binary Interaction Approximation to $N$ -Body Problems

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The binary interaction approximation (BIA) to the  $N$ -body problems is proposed. The BIA conserves total linear momenta in principle. Other invariants, such as the total angular momentum and total energy, are conserved as much effective digits as at least 12 for a two dimensional hydrogen plasma of  $T = 10$  keV and  $n = 10^{20} \text{ m}^{-3}$ . It is found for such a plasma that the total CPU time of the BIA approximately scales as  $N^{1.9}$ .

Keywords:  $N$ -body problem, algebraic approximation, binary interaction approximation, variable step size.

## 1 Introduction

In an isolated  $N$ -body charged particle system as shown in Fig. 1, the non-relativistic equation of motion for the  $i$ -th particle with an electric charge  $q_i$  and a mass  $m_i$  is as follows:

$$m_i \frac{d\mathbf{v}_i}{dt} = q_i \sum_{j \neq i}^N \frac{q_j}{4\pi\epsilon_0} \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}, \quad (1)$$

where  $\mathbf{r}_i$  and  $\mathbf{v}_i$  stand for the position and the velocity of the  $i$ -th particle. Hereafter, the calculation using the above equation of motion Eq. (1) will be referred to as the DIM, direct integration method.

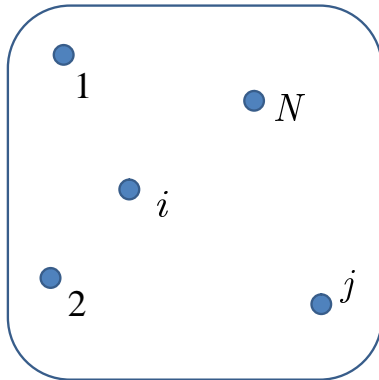


Fig. 1 An  $N$ -body system.

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. However, it is practically impossible for the large number of particles, i.e.  $N \gg 1$ , since the number of force calculations on the right hand side of Eq. (1) is in proportion to  $N^2$ . Moreover, the time step tends to decrease with increasing  $N$ , thus the total CPU time should scale as  $N^3$ .

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The efficient and fast algorithms to calculate interparticle forces include the tree method [1, 2], the fast multipole expansion method (FMM) and the particle-mesh Ewald (PPPM) method [3]. Efforts have been made to use parallel computers, and/or to develop special purpose hardware to calculate interparticle forces, e.g. the GRAPE (GRAVity PipE) project [4]. The authors have recently developed an algebraic model for multibody problems [5], and have shown that the momentum transfer cross-section with our model is in good agreement with the exact one [5, 6]. Unfortunately, this model turns out to lack in enough accuracy in predicting individual particle motion [6].

As shown in Fig. 2 the scattering angle,  $\chi \equiv \pi - 2\theta_0$ , is given by  $b = b_0 \tan \theta_0$ , where  $b$  is the impact parameter,  $b_0 \equiv e^2/4\pi\epsilon_0\mu g_0^2$  corresponds to  $\chi = \pi/2$  scattering, and  $g_0$  the initial relative speed at  $r = \infty$  and  $\theta = -\theta_0$ . In

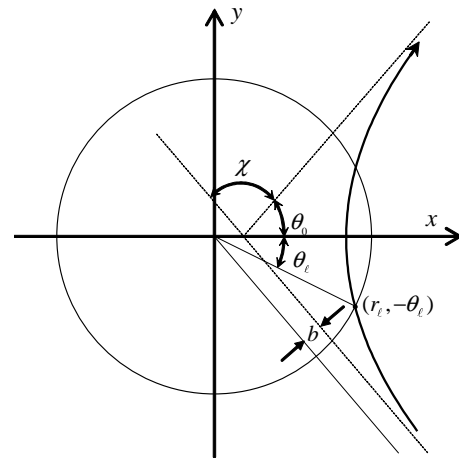


Fig. 2 Unperturbed relative trajectory  $r = r(\theta)$  in an orbital plane. The scattering center is at the origin. An impact parameter is  $b = b_0 \tan \theta_0$ .

the binary system with an impact parameter  $b$ , a typical velocity change  $\Delta g$  in the relative velocity is given by

$$\Delta g = 2g_0 \sin \frac{\chi}{2} \sim \epsilon g_0, \quad \epsilon \equiv \frac{b_0}{\Delta \ell}, \quad (2)$$

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 interaction is of order of  $\epsilon^2$  and can be ignored. It should be noted that the Debye lengths  $\lambda_D$  in fusion plasmas generally satisfy  $\lambda_D \gg \Delta\ell$ , 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.

In this study, we will propose the binary interaction approximation (BIA) to the  $N$ -body systems with  $\epsilon \ll 1$ , and compare it with the direct integration method (DIM), both using the 6-stage 5-th order Runge-Kutta-Fehlberg (RKF65) integrator [7, 8] with an absolute numerical error tolerance of  $10^{-16}$ .

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

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

$$\mu_{ij} \frac{d\mathbf{g}_{ij}}{dt} = \frac{q_i q_j}{4\pi\epsilon_0} \frac{\mathbf{r}_{ij}}{r_{ij}^3} \quad (3)$$

where  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$  stands for the relative position,  $\mathbf{g}_{ij} = \mathbf{v}_i - \mathbf{v}_j$  the relative velocity, and  $\mu_{ij} = m_i m_j / (m_i + m_j)$  the reduced mass. In the BIA, the above equation is integrated, completely ignoring the other particles, from  $t = 0$  to  $t = \Delta t$  to give  $\Delta\mathbf{r}_{ij}$  and  $\Delta\mathbf{g}_{ij}$ . The total number of integration is  ${}_N C_2 = N(N-1)/2$  for an  $N$ -body problem. The individual changes in position  $\Delta\mathbf{r}_i$  and velocity  $\Delta\mathbf{v}_i$  of

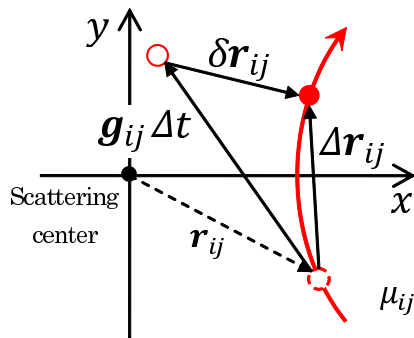


Fig. 3 Relative motion for the particle pair of  $(i, j)$ . A scattering center is at the origin. The change in position of the particle with a mass  $\mu$  is  $\Delta\mathbf{r}_{ij}$ . If there is no interaction, the change in position is  $\mathbf{g}_{ij}\Delta t$  during a time interval of  $\Delta t$ .

the  $i$ -th particle are as follows

$$m_i \Delta\mathbf{r}_i = m_i \mathbf{v}_i \Delta t + \sum_{j \neq i}^N \mu_{ij} (\Delta\mathbf{r}_{ij} - \mathbf{g}_{ij} \Delta t) \quad (4)$$

$$m_i \Delta\mathbf{v}_i = \sum_{j \neq i}^N \mu_{ij} \Delta\mathbf{g}_{ij} \quad (5)$$

for  $i = 1, 2, \dots, N$ . Note that the term within the parentheses, i.e.  $\delta\mathbf{r}_{ij} \equiv \Delta\mathbf{r}_{ij} - \mathbf{g}_{ij}\Delta t$ , on the right hand side of Eq. (4) vanishes when the interaction between the pair  $(i, j)$  vanishes. In other words, the BIA scheme is exact for free particles. It should also be noted that the total momenta  $\mathbf{P} \equiv \sum_{i=1}^N m_i \mathbf{v}_i$  is kept constant with this approximation, since, from Eq. (5) and  $\mu_{ij} = \mu_{ji}$ ,

$$\sum_{i=1}^N m_i \Delta\mathbf{v}_i = \sum_{i=1}^{N-1} \sum_{j=i+1}^N \mu_{ij} (\Delta\mathbf{g}_{ij} + \Delta\mathbf{g}_{ji}) = 0, \quad (6)$$

which also ensures the center of mass position  $\mathbf{R}_{CM}$  to be exact:

$$\mathbf{R}_{CM}(\Delta t) = \mathbf{R}_{CM}(0) + \mathbf{G}_{CM}(0) \Delta t, \quad (7)$$

where  $\mathbf{G}_{CM}$  is the center of mass velocity.

## 3 Calculation

### 3.1 Initial condition for an $N = 122$ -body problem.

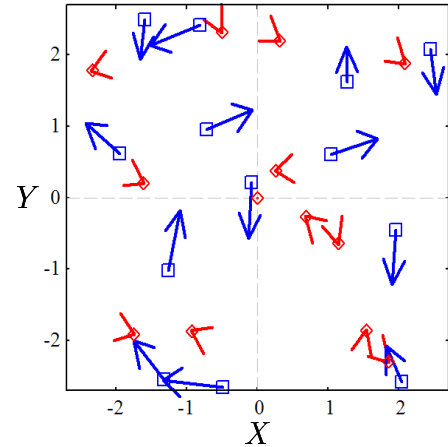


Fig. 4 Initial positions normalized by the interparticle separation  $\Delta\ell \equiv n^{-1/3}$  of an  $N = 122$ -body problem. Only 26 particles near the origin are depicted. Squares with arrows in blue stand for the electron positions and velocities, and diamonds with arrows in red for the protons. Spatial distribution is uniform both for protons and electrons. The Maxwellian velocity distribution is adopted for a given temperature  $T = T_{\text{electron}} = T_{\text{proton}}$ .

Figure 4 depicts the initial condition for a two-dimensional  $N = 122$ -problem, in which there are 61 protons and 61 electrons. Note that only 26 particles near the

origin are depicted in the figure. In this and the following figures, positions are normalized by the interparticle separation  $\Delta\ell \equiv n^{-1/3}$ , and velocities by the relative thermal speed among electrons,  $g_{\text{th}}^{ee} = \sqrt{2}v_{\text{th}}^e$ . Squares with arrows in blue in Fig. 4 stand for the electron positions and velocities, and diamonds with arrows in red for the protons. Spatial distribution is uniform and the velocity distribution is maxwellian for both species with temperatures of  $T = T_{\text{electron}} = T_{\text{proton}} = 10$  keV. The number density  $n = 10^{20} \text{ m}^{-3}$  is assumed, which leads to the parameter  $\epsilon = 1.67 \times 10^{-7} \ll 1$ .

### 3.2 Trajectories of a proton and an electron.

The 122-body system is integrated for  $\Delta t \equiv \Delta\ell/g_{\text{th}}^{ee}$ , i.e. the time for the electron with its thermal speed to travel the average interparticle separation  $\Delta\ell \equiv n^{-1/3}$ . Figures 5 and 6 show the trajectories in the configuration space  $(X, Y)$  on the left and velocity space  $(U, V)$  on the right for a proton initially at rest, and a moving electron, respectively. In both figures, the diamonds labeled 'initial' are initial points at  $t = 0$ . The lines are trajectories solved by using the DIM. Triangles indicate the final points at  $t = \Delta t$  by the BIA. The agreement between the BIA and the DIM is excellent.

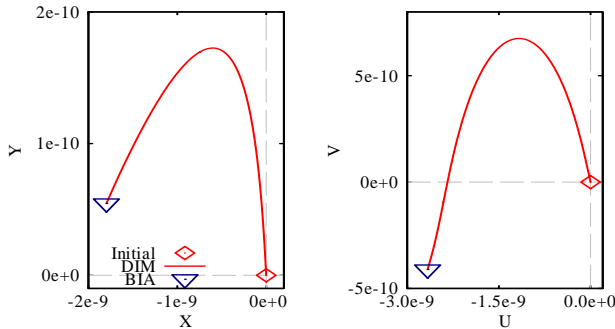


Fig. 5 A proton motion initially at rest in the configuration space on the left, and in the velocity space on the right, for the  $N = 122$ -body system. Symbols represent the initial and final position calculated by the BIA. The particle starting at the diamonds goes along lines which are calculated by the full  $N$ -body integration, i.e. the DIM.

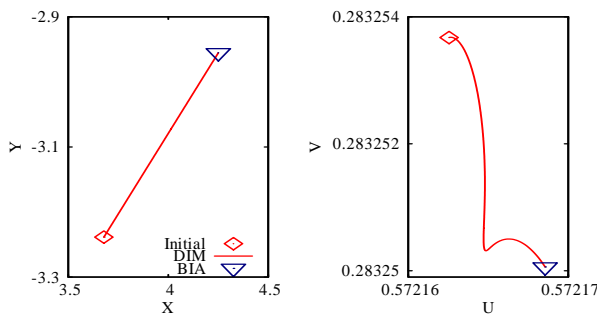


Fig. 6 An electron motion for the  $N = 122$ -body system. Legends are the same as Fig. 5.

As is typically seen on the right in Fig. (6), the com-

puted velocity change in time, or the acceleration, is reproduced well by the BIA, in which three-or-more body interactions are ignored.

### 3.3 Errors and effective digits of invariants.

There are four invariants of motion in an isolated two dimensional system; the total linear momenta  $\mathbf{P}$ , the total angular momentum  $L_Z$ , and the total energy  $E$ . Effective digits for calculated invariants of motion and CPU time for  $N = 122$  are listed in Table 1, in which, with  $\mathbf{r}_i = (X_i, Y_i)$  and  $\mathbf{v}_i = (U_i, V_i)$ ,

$$P_X = \sum_{i=1}^N m_i U_i, \quad (8)$$

$$P_Y = \sum_{i=1}^N m_i V_i, \quad (9)$$

are the total linear momenta,

$$L_Z = \sum_{i=1}^N m_i (X_i V_i - Y_i U_i), \quad (10)$$

the total angular momentum, and

$$E = \frac{1}{2} \sum_{i=1}^N m_i v_i^2 + \frac{1}{4\pi\epsilon_0} \sum_{i=1}^{N-1} q_i \sum_{j=i+1}^N \frac{q_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (11)$$

the total energy of the system.

Table 1 Effective digits for calculated invariants of motion and CPU time for  $N = 122$ .  $P_X$  and  $P_Y$  are the total linear momenta,  $L_Z$  the total angular momentum,  $E$  the total energy of the system.

method	$P_X$	$P_Y$	$L_Z$	$E$	CPU time
DIM	16	15	16	16	3.4
BIA	16	15	15	12	0.2
unit	digit				sec

Note that the effective digits of 15-16 is the maximum for 64-bit calculation on the computer used in this study. In the case of the DIM, all the effective digits for invariants reach this maximum, while the total energy conservation for the BIA is 12 digits, worse than the DIM which is generally the case. The angular momentum conservation for the BIA happens to be 15 digits for this particular initial conditions for  $N = 122$ -body problem. The conservation in  $L_Z$ , however, is generally close to that in  $E$  for different initial conditions and the number of particles  $N$ .

As for the CPU time, the BIA is 17 times faster than the conventional DIM for  $N = 122$ . Since the speed up ratio depends essentially on the number of particles  $N$ , calculations for different  $N$  will be examined in the following subsection.

### 3.4 CPU time dependence on $N$

We made similar calculation to the foregoing section varying the number of particles,  $N$ . The CPU time dependence on  $N$  with fitting lines are depicted in Fig. 7, in which CPU time inversions are found for the DIM, i.e. longer CPU time  $\tau_{\text{DIM}}^{\text{CPU}}(N) > \tau_{\text{DIM}}^{\text{CPU}}(N')$  for less number of particles  $N < N'$  at around  $N \sim 700$  and  $1600$ . Such inversions can occur because the integrator RKF65 used here controls the time step size during the calculation according to the given error tolerance. The CPU time for the direct integration method scales as  $\tau_{\text{DIM}}^{\text{CPU}} \propto N^{2.7}$ , and the binary interaction approximation  $\tau_{\text{BIA}}^{\text{CPU}} \propto N^{1.9}$  both using the RKF65 with the same absolute error tolerance of  $10^{-16}$ . Also BIA 1 is the CPU time to calculate only one particle, which scale as  $\tau_{\text{BIA1}}^{\text{CPU}} \propto N^{1.0}$ . If we are interested in motion of only one test particle- $i$  at a time  $t = \Delta t$  from initial conditions at  $t = 0$ , it is possible with the BIA to calculate  $\mathbf{r}(\Delta t)$  and  $\mathbf{v}(\Delta t)$ , since it is based on the principle of superposition of  $\Delta \mathbf{r}_{ij}$  and  $\Delta \mathbf{v}_{ij}$  using Eqs. (5) and (4).

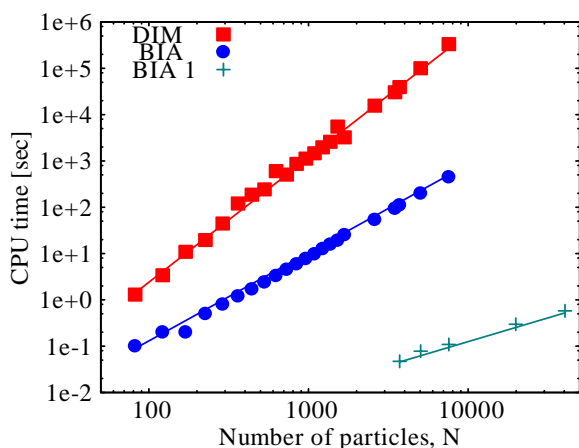


Fig. 7 CPU time  $\tau^{\text{CPU}}$  dependence on the number of particles  $N$  on a typical PC. Red squares stand for the CPU time for the DIM with a fitting line in red,  $\tau_{\text{DIM}}^{\text{CPU}} \propto N^{2.7}$ . Blue circles stand for the CPU time for the BIA with a fitting line in blue,  $\tau_{\text{BIA}}^{\text{CPU}} \propto N^{1.9}$ . Also BIA 1 is the CPU time to calculate only one particle, which scale as  $\tau_{\text{BIA1}}^{\text{CPU}} \propto N^{1.0}$ .

As was shown on the right in Fig. 6, the temporal electron acceleration is complicated due to its small mass. For a given numerical error tolerance, this tends to make the common time step smaller, and consequently make the total CPU time  $\tau^{\text{CPU}}$  longer especially in the DIM. On the other hand, the BIA with the same error tolerance as the DIM is a *pair wise* variable time step scheme, since the time step for the pair  $(i, j)$  is independent from that for any other pairs  $(i, j')$ .

## 4 Summary and Discussion

The binary interaction approximation, the BIA, to the  $N$ -body problems is proposed. 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 [7, 8]. Other invariants, such as the total angular momentum and total energy, are conserved as much effective digits as at least 12 for a two dimensional hydrogen plasma of  $T = 10$  keV and  $n = 10^{20} \text{ m}^{-3}$ , in which  $\epsilon \sim 1.67 \times 10^{-7}$ . The CPU time of the BIA scales as  $\tau_{\text{BIA}}^{\text{CPU}} \propto N^{1.9}$  for such a plasma. It should also be noted that with the BIA it is possible to calculate only one particle's motion [6] with the CPU time in proportion to  $N$ .

The numerical results presented here is for two dimensional systems with low density and high temperature, i.e.  $\epsilon \ll 1$ , which is the most appropriate for the BIA. We will soon apply the BIA to three dimensional cases, and/or to systems with  $\epsilon \sim 1$ , such as the gravitational  $N$ -body systems, in the near future.

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