Algebraic Analysis Approach for Multibody Problems II

Shun-ichi OIKAWA, Koichiro HIGASHI and Hideo FUNASAKA[a)]

Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan

(Received 6 January 2009 / Accepted 8 June 2009)

The algebraic model (ALG) proposed by the authors has sufficiently high accuracy in calculating the motion of a test particle with all the field particles at rest. When all the field particles are moving, however, the ALG has relatively poor prediction ability on the motion of the test particle initially at rest. None the less, the ALG approximation gives a good results for the statistical quantities, such as variance of velocity changes or the scattering cross section, for a sufficiently large number of Monte Carlo trials. For a 10^8-body problem, which corresponds to full three-dimensional Coulomb interactions within the Debye sphere in a fusion plasma, the ALG approximation is 263 times as fast as the 6-stage 5-th order Runge-Kutta-Fehlberg method with an absolute error tolerance of 10^{-16}.

Keywords: multibody problem, algebraic approximation, binary interaction approximation, direct integration method

DOI: 10.1585/pfr.5.S1048

1. Introduction

Since it is difficult to rigorously deal with multibody Coulomb and gravitational collisions, the current classical theory considers them as a series of temporally-isolated binary Coulomb and gravitational collisions within the Debye sphere. The efficient and fast algorithms to calculate inter-particle forces include the tree method [1, 2], the fast multipole expansion method (FMM) and the particle-mesh Ewalt (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]. Some of the authors have developed an algebraic model for multibody problems, and have shown that the momentum transfer cross-section with our model is in good agreement with the exact one [5].

As shown in Fig. 1 the scattering angle, $\chi \equiv \pi - 2\theta_0$, is given by $b = b_0 \tan\theta_0$, where b is the impact parameter, $b_0 \equiv e^2/4\pi\varepsilon_0\mu g_0^2$ corresponds to $\chi = \pi/2$ scattering, and g_0 the initial relative speed at $r = \infty$ and $\theta = -\theta_0$. The angular component of the equation motion gives the well-known invariant of

$$r^2 \frac{\mathrm{d}\theta}{\mathrm{d}t} = \text{const} = b g_0, \tag{1}$$

and the radial component is given by

$$\frac{\mathrm{d}^2 r}{\mathrm{d}t^2} = \frac{g_0^2 b_0}{r^2}\left(1 + \frac{b_0}{r}\tan^2\theta_0\right), \tag{2}$$

which can be analytically solved as

$$r(\theta) = \frac{b\sin\theta_0}{\cos\theta - \cos\theta_0}.$$

The first term in the parentheses on the right hand side of Eq. (2) stands for the Coulomb force $F_\mathrm{c} \propto r^{-2}$. This force is much smaller for small angle scatterings, i.e. $\chi \ll 1$, than the second term F_a which scales as $\propto r^{-3}$ and results from the conservation of angular momentum Eq. (1), since, at the closest point $r_\mathrm{min} = r(\theta = 0)$ shown in Fig. 1, we have

$$\frac{b_0 \tan^2\theta_0}{r_\mathrm{min}} \simeq \frac{2}{\chi} \gg 1. \tag{3}$$

Thus the main force on the particle is not the Coulomb force F_c, but F_a due to the conservation of angular momentum.

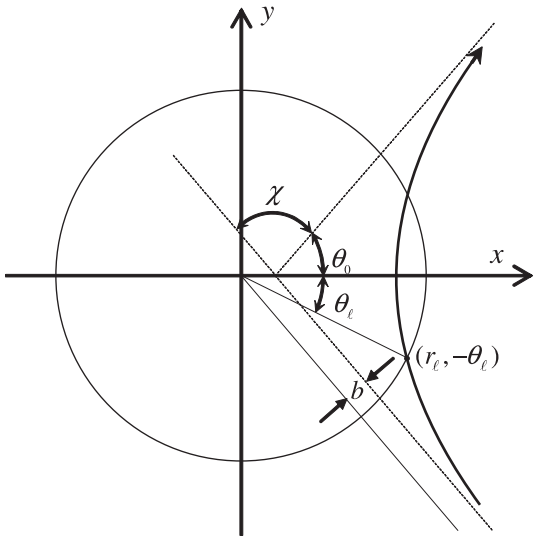

Fig. 1 Unperturbed relative trajectory $r = r(\theta)$ in an orbital plane for the repulsive force. The scattering center is at the origin. An impact parameter is $b = b_0 \tan\theta_0$. Interaction region is inside the circle with a radius $r_\ell = \Delta\ell/2$, where $\Delta\ell$ stands for the average interparticle separation.

author's e-mail: oikawa@qe.eng.qe.hokudai.ac.jp

[a)] currently with DENSO Corporation

2. Algebraic Approximation

Since the r-dependence on $F_a \propto r^{-3}$ is steeper than that on $F_c \propto r^{-2}$, the momentum change in $\mu \boldsymbol{g}$ is almost due solely to F_a near $r = r_{min}$. As a consequence, the exact hyperbolic trajectory for the particle can be approximated as a broken line with an impulse force of

$$\mu \Delta \boldsymbol{g} = 2\mu g_0 \cos\theta_0 \boldsymbol{e}_x, \tag{4}$$

near the closest point as shown in Fig. 2.

With this in mind, we have approximated a multibody problem to a series of binary deflections near their closest point as shown in Fig. 2, in which a test particle starts at the lower-right point, and its final point is at the upper-right point due to the interaction with a field particle at rest.

2.1 Coordinate transformation

In order to apply the above binary interaction approximation (ALG) shown in Fig. 2 to multibody cases, first we seek for a field particle that gives the test particle an impulse force *at the earliest time*. For this purpose, it is convenient to transform the coordinate system from (x, y) to (ξ, η), in such a way that the initial position of the test particle is at the origin $(\xi, \eta) = (0, 0)$ and the relative velocity $\boldsymbol{g} \equiv \boldsymbol{v}_i - \boldsymbol{v}_j$ is $(g_\xi, g_\eta) = (0, g)$. Then the relative position $\boldsymbol{r} \equiv \boldsymbol{r}_i - \boldsymbol{r}_j$ has an η-coordinate of

$$\eta_{ij} = \frac{\boldsymbol{r} \cdot \boldsymbol{g}}{g}. \tag{5}$$

The particle moves along the η-axis with a constant velocity of g, and is to interact at $\left(0, \eta_{ij}\right)$ with this field particle in a time interval of $\Delta t_{ij} \equiv \eta_{ij}/g$ sec. Accordingly, the field particle that the test particle is given an impulse force at the earliest time has the smallest positive η_{ij}, i.e.

$$\eta_{min} \equiv \min(\max(0, \eta_{ij})), \text{ for } 1 \le i, j \le N. \tag{6}$$

We have ignored the effect of field particles with $\eta_{ij} < 0$, since the interaction is completed at $\eta = 0$ in our approximation. In other words, such field particles have already interacted with the test particle in the past.

When the test particle moves to the position of $(0, \eta_{min})$, it changes the relative velocity by $\Delta \boldsymbol{g}_{ij}$ as

$$\Delta \boldsymbol{g}_{ij} = -2g \sin\frac{\chi_{ij}}{2} \boldsymbol{e}_\xi, \tag{7}$$

$$\chi_{ij} \simeq 2 \arctan\frac{b_0}{\xi_{ij}}, \tag{8}$$

where the pair i and j satisfies Eq. (6), and we have approximated that the impact parameter is given by $b = \xi_{ij}$ in Eq. (4) as shown in Fig. 3. Thus, in the (ξ, η) coordinate system, the field particle position ξ_{ij} and η_{ij} correspond to the velocity change $\Delta \boldsymbol{g}_{ij}$ and the time of the interaction Δt_{ij}, respectively. This procedure will be repeated until the test particle leaves the prescribed interaction region, i.e. $r < \Delta\ell/2$ as depicted in Fig. 1.

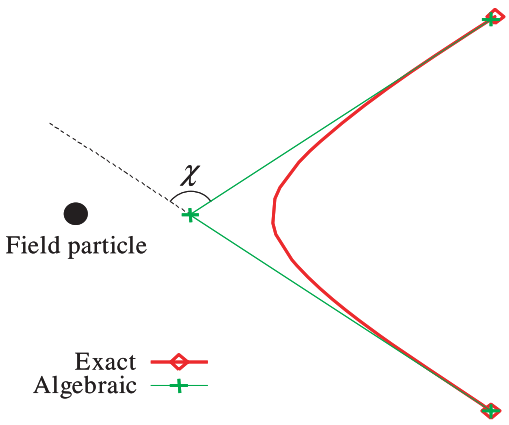

Fig. 2 Algebraic trajectory (broken line) and exact trajectory (curved line) which is a part of a hyperbola. A field particle (black circle) is on the left.

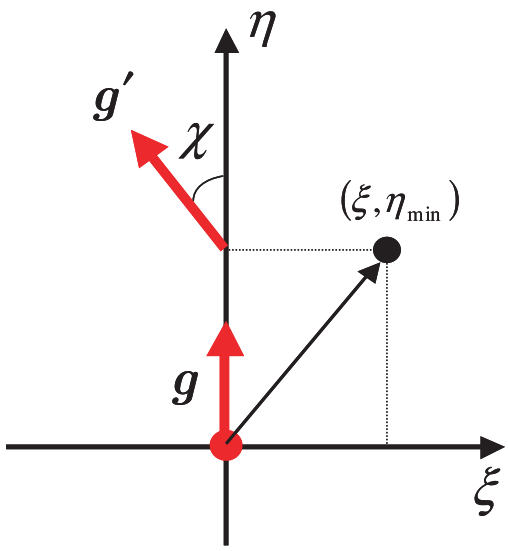

Fig. 3 Coordinate transform from the (x, y) to (ξ, η). In this coordinate system, the scattering angle χ, i.e. the impact parameter b and the time of the interaction Δt are approximately given by ξ and η, respectively. The relative velocity at $t = 0$ is $\boldsymbol{g}$, and is $\boldsymbol{g}' = \boldsymbol{g} + \Delta \boldsymbol{g}$ at $t = \Delta t$.

3. Calculation

The numerical results with using the *direct integration method*, DIM, hereafter refers to that obtained by solving the following equation of motion a particle-i with a charge q_i, a mass m_i, and velocity $\boldsymbol{v}_i$ at a position $\boldsymbol{r}_i$

$$m_i \frac{\mathrm{d}\boldsymbol{v}_i}{\mathrm{d}t} = q_i \sum_{j \ne i}^{N} \frac{q_j}{4\pi\varepsilon_0} \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|^3}. \tag{9}$$

As the DIM in this study, we will use the 6-stage 5-th order Runge-Kutta-Fehlberg method known as the RKF65 [7, 8] with the absolute numerical error tolerance of 10^{-16}.

In the following calculations, we will assume that, except the test particle, the field particles on the average are randomly distributed in the phase space $(\boldsymbol{r}, \boldsymbol{v})$. In configuration space, field particles are distributed with the average

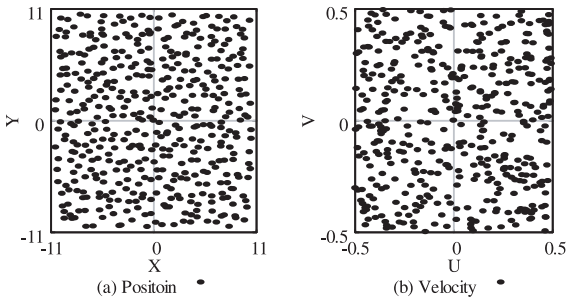

Fig. 4 The typical initial conditions of particles; (a) positions normalized by the interparticle separation on the left, and (b) in the particle velocity normalized by the thermal speed on the right. The number of particles is 422.

interparticle separation, $\Delta\ell$. We will consider two cases: all the field particles are fixed at their initial positions, the Case 1, and moving field particles, the Case 2. The typical initial condition is depicted in Fig. 4. The numerical conditions correspond to a fusion plasma with a temperature of $T = 10$ keV and a number density of $n = 10^{20}$ m^{-3}. In such plasmas, the Debye length is $\lambda_D \sim 500\Delta\ell$, where $\Delta\ell \equiv n^{-1/3}$.

3.1 Case 1: All field particles at rest

In the Case 1, all the field particles are at rest, and one of them locates at the origin. The test particle starts from the position of $(b, -\Delta\ell/2)$ with a velocity of $(0, v_0)$. Thus b is the impact parameter against the field particle initially at the origin.

Figure 5 is an example out of 10^5 Monte Carlo calculations for an impact parameter $b = 0.3\Delta\ell$, and compares the algebraic (ALG) trajectory and the exact (DIM) trajectory normalized by the interparticle separation $\Delta\ell$. Note that the DIM results are accurate up to of the order of 10^{-16} which is the absolute error tolerance adopted. The circles in the figure indicate the positions at which the test particle is given the impulse force by one of 441 field particles. The algebraic (ALG) approximation agrees well with the direct integration method, DIM, in most cases as shown in Fig. 5.

Depicted in Fig. 6 is the *accumulated* scattering cross section $\sigma_{\rm acc}(b)$ as a function of the impact parameter b defined by

$$\sigma_{\rm acc}(b) = \int_0^b \left(\frac{\Delta g}{g}\right)^2 \pi b\, {\rm d}b \approx \frac{\pi(\Delta t)^2}{10^3} \sum_{k=1}^{10^3 b/\Delta\ell} k \times \left\langle (\Delta g_k)^2 \right\rangle, \qquad (10)$$

where $\left\langle (\Delta g_k)^2 \right\rangle$ is the variance for the impact parameter $b_k = k\times\Delta\ell/10^3$ with a Monte Carlo trials of 10^5 adopted in this study. The agreement of $\sigma_{\rm acc}^{\rm ALG}(b)$ with the exact one, $\sigma_{\rm acc}^{\rm DIM}(b)$, is also excellent. It should, however, be noted that all the field particles are at rest throughout the calculation in this case [5].

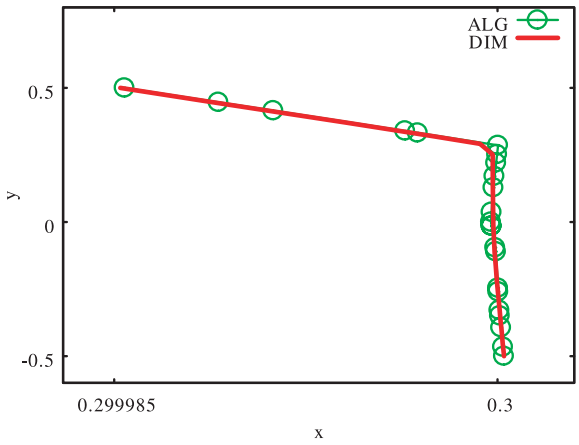

Fig. 5 Comparison of algebraic trajectory (denoted by ALG) and the exact trajectory (denoted by DIM, direct integration method) in the case of two-dimensional 442-body Coulomb collisions with an impact parameter $b = 0.3\Delta\ell$. Coordinates (x, y) are normalized by $\Delta\ell$. The circles in the figures for the algebraic trajectories stand for the positions at which the test particle is given the impulse force by one of 441 field particles.

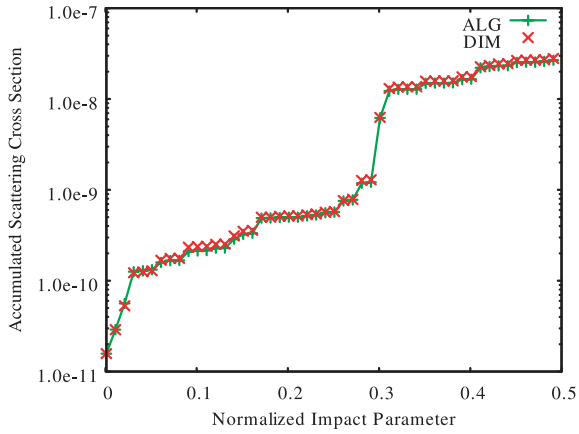

Fig. 6 Accumulated Coulomb scattering cross section normalized by the square of the average interparticle separation, $\sigma_{\rm acc}(b)/\Delta\ell^2$, vs normalized impact parameter $\bar{b} = b/\Delta\ell$ in the case of $N = 442$-body. See Ref. [5] for detail.

The two-dimensional total multibody scattering cross section for $b = b_{\rm max} = \Delta\ell/2$ in Fig. 6 ,

$$\sigma_{\rm acc}(b_{\rm max} = \Delta\ell/2) \sim 2.8\times10^{-8}\times\Delta\ell^2, \qquad (11)$$

is more than 10^3 times the conventional binary cross section [9, 10],

$$\sigma_{\rm bin} = 4\pi b_0^2 \ln\frac{b_{\rm max}}{b_0} \sim 2.3\times10^{-11}\times\Delta\ell^2, \qquad (12)$$

with the maximum impact parameter $b_{\rm max} = \Delta\ell/2$. As pointed out in Ref. [5], however, this is not the anomalous diffusion. The binary interaction occurs in an orbital plane, whereas multibody interactions are inherently three-dimensional. Even if a field particle locates so close to the

test particle in the (x, y) plane that the interaction results in a large angle scattering in the 2-d calculation with, say, $z = 0$, the same field particle locates not necessarily close to the test particle with $z \neq 0$ in 3-d.

The CPU time required for the algebraic approximation is only about 20 min using a personal computer, whereas the exact analysis requires 15 hours to integrate the entire set of multibody equations of motion, i.e. the DIM.

3.2 Case 2: Moving field particles.

Strictly speaking, the Case 1 does not deal with the multibody problem, but solves the test particle motion in the presence of the multiple field particles at rest. In the Case 2, we will loosen the above restriction on the field particle motion, and have applied the algebraic model to the 442-body problem, in which there are 441 moving field particles and a test particle initially at rest. The two-dimensional 442-body system is analyzed for the time interval $\Delta t \equiv \Delta\ell/g_{\rm th}$, i.e. the time for a particle with a thermal speed $g_{\rm th}$ to travel the interparticle separation $\Delta\ell = n^{-1/3}$.

The change in position $\Delta \boldsymbol{r}$ (results not shown) of the field particles during the time interval Δt are in good agreement with the exact one, since they are moving in a very weak potential so that $\Delta \boldsymbol{r}_i \sim \boldsymbol{v}_i(0)\,\Delta t$ to a good approximation. Although, the absolute value of the change in velocity $|\Delta \boldsymbol{v}|$ of each particle by the ALG are of the same order as the exact one, the orientation of $\Delta \boldsymbol{v}$ is not correct as shown in Fig. 7, where the test particle starts at the upper-right point $(U, V) = (0, 0)$. Also depicted for reference in Fig. 7 is the final point at $t = \Delta t$ by using the BIA, the binary interaction approximation, proposed by the authors [6]. Note that the BIA accurately predicts the final point of the DIM with the absolute error tolerance of 10^{-16}.

In spite of relatively poor accuracy in the individual particle motion, the ALG approximation still gives a good result for the statistical quantities, such as variance of velocity changes for a large number of Monte Carlo trials, $N_{\rm MC}$. The green circles in Fig. 8 for the ALG show the variance of changes in normalized velocity, $\left\langle (\Delta \boldsymbol{v})^2 \right\rangle / g_{\rm th}^2$, of the test particle initially at rest as a function of the number of the Monte Carlo trials $N_{\rm MC}$, in which the variance up to $N_{\rm MC} = 10^4$ with red line by using the DIM is also shown. Several jumps seen in Fig. 8 are due to close encounters, i.e. large angle scatterings with $\Delta v_{\rm i}/g_{\rm th} \sim 1$. At the number of Monte Carlo trials $N_{\rm MC} = 10^4$, the normalized variance by using the ALG, $\left\langle (\Delta \boldsymbol{v})^2 \right\rangle = 2.016 \times 10^{-8} \times g_{\rm th}^2$, agrees with that due to the DIM, $\left\langle (\Delta \boldsymbol{v})^2 \right\rangle = 2.022 \times 10^{-8} \times g_{\rm th}^2$, within a relative error less than 0.3 %. As will be shown in Fig. 9 on the CPU times, the DIM for $N_{\rm MC} = 10^6$ Monte Carlo trials would need a CPU time $\tau_{\rm DIM}^{\rm CPU} \sim 10^8$ sec ~ 3 years, while only 2×10^4 sec ~ 6 hours for the ALG, both on a personal computer (Intel Pentium 4, 2.60C GHz).

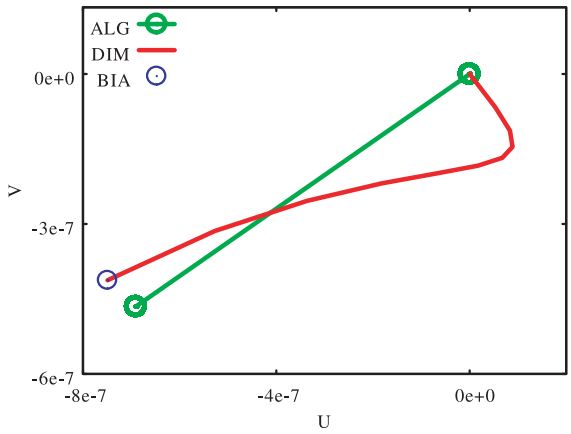

Fig. 7 Case 2: Trajectory of the test particle initially ($t = 0$) at rest, in the velocity space (U, V) normalized by the thermal speed g_{th}. There are 441 moving field particles. The final point at $t = \Delta t$ calculated by using the binary interaction approximation, the BIA [6], is also shown.

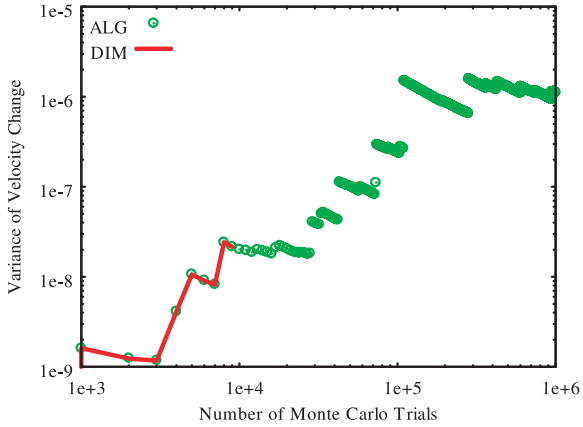

Fig. 8 Variance of the change in velocity, $\left\langle (\Delta \boldsymbol{v})^2 \right\rangle / g_{\rm th}^2$, of the test particle initially at rest, in the case of $N = 442$-body; the Case 2. There are no data for the DIM beyond the Monte Carlo trials $N_{\rm MC} = 10^4$, since the DIM calculation needs much time for larger $N_{\rm MC}$.

3.3 Comparison of CPU times

In the case of moving field particles as the Case 2, the CPU time $\tau^{\rm CPU}$ dependence on the number of particles $N = 442,\ 841,\ 1682,\ 3722,\ 10202$, and 20450 is examined on the personal computer.

The red squares in Fig. 9 stand for the CPU time of the DIM with the red fitting line of

$$\tau_{\rm DIM}^{\rm CPU}(N) \sim 2.06 \times 10^{-6} \times N^{2.83} \text{ sec.} \tag{13}$$

Note that the DIM for $N = 20450$ was not examined since it would take a CPU time of the order of 37 days. The green triangles in Fig. 9 represent the ALG with the green fitting line of

$$\tau_{\rm ALG}^{\rm CPU}(N) \sim 2.36 \times 10^{-10} \times N^{3.02} \text{ sec,} \tag{14}$$

and the blue circles for the BIA with the fitting line in blue, $\tau_{\rm BIA}^{\rm CPU} \sim 5.04 \times 10^{-6} \times N^{1.99}$ sec. Thus, from Eqs. (13) and

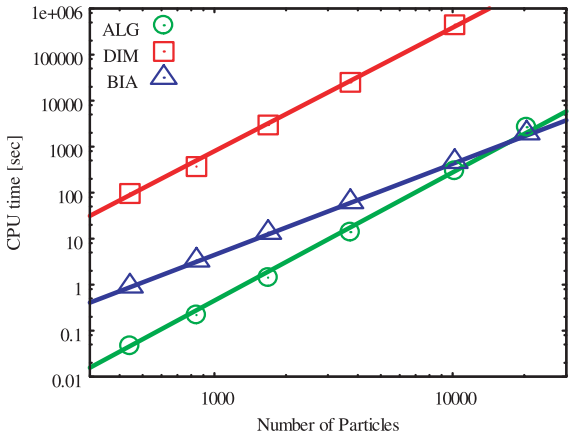

Fig. 9 CPU time $\tau^{\rm CPU}$ dependence on the number of particles N = 442, 841, 1682, 3722, 10202, and 20450, on a typical PC (Intel Pentium 4, 2.60C GHz). Red squares stand for the CPU time for the DIM with a fitting line in red, $\tau^{\rm CPU}_{\rm DIM} \propto N^{2.83}$. Green triangles stand for the CPU time for the ALG with a fitting line in green, $\tau^{\rm CPU}_{\rm ALG} \propto N^{3.02}$. Blue circles stand for the CPU time for the BIA with a fitting line in blue, $\tau^{\rm CPU}_{\rm BIA} \propto N^{1.99}$.

(14), the ALG scheme calculates the variance of velocity changes $8.73\times10^3\times N^{-0.19}$ times as fast as the DIM, specifically the RKF65 method in this study. In other words, the ALG is faster than the DIM for the number of particle N less than 5.5×10^{20}. For a 10^8-body problem, which corresponds to full three-dimensional Coulomb interactions within the Debye sphere in a fusion plasma, the ALG approximation would still be 2.63×10^2 times as fast as the DIM.

4. Conclusion

The algebraic model (ALG) proposed by the authors has sufficiently high accuracy in calculating the motion of a test particle with all the field particles at rest. When all the field particles are moving, however, the ALG has relatively poor prediction ability on the motion of the test particle initially at rest. None the less, the ALG approximation gives good results for the statistical quantities, such as variance of velocity changes, i.e. the scattering cross section, for a sufficiently large number of Monte Carlo trials. The CPU time of the approximation is $8.73\times10^3\times N^{-0.19}$ times shorter than the 6-stage 5-th order Runge-Kutta-Fehlberg method with an absolute error tolerance of 10^{-16}.

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

Acknowledgement

The authors would like to thank Dr. A. Wakasa, Prof. Y. Matsumoto and Prof. M. Itagaki for their fruitful discussions on the subject. The author would also acknowledge the continuous encouragement of the late Prof. T. Yamashina. This research was partially supported by a Grant-in-Aid for Scientific Research (C), 21560061 from the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

[1] A. W. Appel, SIAM J. Sci. Stat. Comput. **6**, 85 (1985).
[2] J. E. Barnes and P. Hutt, Nature **324**, 446 (1986).
[3] P. P. Brieu, F. J. Summers and J. P. Ostriker, APJ **453**, 566 (1995).
[4] J. Makino and M. Taiji, APJ **480**, 432 (1997).
[5] S. Oikawa and H. Funasaka, Plasma Fusion Res. **3**, S1073 (2008).
[6] S. Oikawa, H. Funasaka, K. Higashi and Y. Kitagawa, *Binary Interaction Approximation to N-Body Problems*, to be appeared in Plasma Fusion Res. **4** (2009).
[7] E. Fehlberg, NASA Technical Report 315 (1969).
[8] E. Fehlberg, *Klassische Runge-Kutta-Formeln vierter und niedrigerer Ordnung mit Schrittweiten-Kontrolle und ihre Anwendung auf Warmeleitungsprobleme*, *Computing* (Arch. Elektron. Rechnen), vol. 6, (1970) pp. 61–71.
[9] R. S. Cohen, L. Spitzer, Jr., and P. McR. Routly, Phys. Rev. **80**, 230 (1950).
[10] W. M. Stacey, Jr., *FUSION PLASMA ANALYSIS*, (Krieger, Malabar, 1992).