Accuracy Assurance in Binary Interaction Approximation for N-Body Problems

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(Received 6 December 2011 / Accepted 1 June 2012)

Two accuracy assurance schemes are combined into the Binary Interaction Approximation (BIA) to N-body problems. The first one is a sort of variable time step (VTS) scheme for a given error tolerance. Since this scheme sometimes does not converge, an error-tolerance-adjusting (ETA) scheme is also introduced. With these two schemes combined into the original BIA, a significant improvement in terms of numerical error is obtained.

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Keywords: binary interaction approximation, N-body problem, accuracy assurance, variable time step scheme, error tolerance adjustment, Runge-Kutta-Fehlberg

DOI: 10.1585/pfr.7.2401103

1. Introduction

We have proposed the Binary Interaction Approximation (BIA) scheme [1–3] to N-body problem. The BIA scheme views an N-body problem as the superposition of \( N^2 \) two-body problems [1]. If we are interested in the motion of only one test particle-\( i \) at a time \( \Delta t \) from initial conditions at \( t = 0 \), it is possible with the BIA scheme to calculate \( r_i(\Delta t) \) and \( v_i(\Delta t) \) completely in parallel.

When the time interval \( \Delta t \) is chosen to be the time \( \Delta t/g_{ib} \) for a particle with a mass \( m \) and its thermal speed of \( g_{ib} = \sqrt{2T/m} \) to travel the average interparticle separation of \( \Delta r = n^{-1/3} \) for plasmas with a temperature \( T \) and a number density \( n \), the BIA is proven to be a powerful scheme for N-body problems [1]. Generally speaking, the BIA scheme is best suitable for fusion plasmas that are low-density and high-temperature gases. As will be shown later, however, for much longer time interval the calculations on the right-hand side of Eq. (1) is in proportion of \( \Delta t/g_{ib} = n^{-2/3} \). The equation of motion for this case, instead of Eq. (1), is:

\[
\frac{dm_i}{dt} = \frac{Z\mu_i e^2}{4\pi\epsilon_0} \sum_{j \neq i} \frac{N_j}{|r_j - r_i|}.
\]

It is practically impossible to deal with 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 number of time-steps tends to increase with increasing \( N \), so the total CPU time should scale as \( N^{2.3} \).

The efficient, fast algorithms to calculate interparticle forces include the tree method [4, 5], the fast multipole expansion method (FMM), and the particle-mesh Ewald (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. BIA Scheme

Fig. 1 A test calculation for a 1,332-body problem. A particle starts at the point marked with a filled circle in green moves in the velocity space (\( u, v, w \)) along a red line, which is obtained by using a direct integration method (DIM), specifically a Runge-Kutta-Fehlberg scheme with an absolute error tolerance of \( 10^{-16} \). The BIA gives the velocity at blue circle, which is close to the endpoint of the red line.

1) This article is based on the presentation at the 21st International Toki Conference (ITC21).

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mass, $Z_i e$ is the electric charge of particle-$i$.

Since the exact solutions to two-body problems are known, for any time interval $\Delta t$ the solution, $r_i(\Delta t)$ and $g_i(\Delta t)$ are easily found from the initial conditions $r_i(0)$ and $g_i(0)$. Once the solutions to all the two-body systems are found, changes in position and in velocity of individual particle during the time interval $\Delta t$ is calculated as follows (see Appendix):

$$m_i \Delta r_i = m_i v_i \Delta t + \sum_{j \neq i}^N \mu_{ij} (\Delta r_{ij} - g_{ij} \Delta t),$$

(3)  

$$m_i \Delta v_i = \sum_{j \neq i}^N \mu_{ij} \Delta g_{ij}.$$  

(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 $\Delta v_i$, changes in position $\Delta r_i$ due to particle $j$ is not simple summation over $\Delta r_{ij}$. As shown in Fig. 2, the subtraction by $g_{ij} \Delta t$ from total change in position $\Delta r_{ij}$ 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).

If we are interested in the motion of only one test particle-$i$ at a time $t = \Delta t$ from the initial conditions at a time $t = 0$, it is possible with the BIA scheme to calculate $r_i(\Delta t)$ and $v_i(\Delta t)$ completely in parallel, since it is based on the principle of superposition of $\Delta r_{ij}$ and $\Delta g_{ij}$ using Eq. (3), and Eq. (4).

As shown in Fig. 1, the complicated change in velocity with time, or the acceleration, is typically reproduced well with the BIA (blue triangle) for a time interval of $1 \times \Delta t = \Delta t / q_0$. For much longer time-interval of $100 \times \Delta t$, the red line in Fig. 3 represents the trajectory calculated by using a Runge-Kutta-Fehlberg integrator [8] with an absolute error tolerance of $10^{-16}$. Note that the BIA scheme gives only the final solution at a given time interval, $100 \times \Delta t$ in this case, from the initial conditions. The final point due to the BIA calculation apparently deviates from that of the DIM. In the following section, we will introduce accuracy assurance schemes to the BIA to reduce the errors, or the deviation from the DIM.

3. Accuracy Assured BIA Scheme

Suppose a general ordinary differential equation, for a time-dependent function $y = y(t)$, of the form:

$$\frac{dy}{dt} = f(y, t),$$

(5)

with an initial condition at a time $t = 0$ of

$$y(0) = y_0.$$  

(6)

Let us define an exact time-shift operator $\mathcal{D}[y, \Delta t]$ on any time-dependent quantity:

$$\mathcal{D}[y(t), \Delta t] \equiv y(t + \Delta t).$$  

(7)

Similarly let us introduce an operator:

$$\mathcal{B}[r_i, \Delta t] = r_i + v_i \Delta t + \frac{1}{m_i} \sum_{j \neq i}^N \mu_{ij} (\Delta r_{ij} - g_{ij} \Delta t)$$

$$\mathcal{B}[v_i, \Delta t] = v_i + \frac{1}{m_i} \sum_{j \neq i}^N \mu_{ij} \Delta g_{ij}$$

(8)

which is an approximate operator to the exact operator $\mathcal{D}[y, t]$ with the BIA scheme described in the foregoing section, i.e. Eqs. (3)–(4).

3.1 Variable-time-step scheme

With these notations defined above, let $y_1(\Delta t)$ and $y_2(\Delta t)$ denote the approximate solutions at a time $t = \Delta t,$
and the velocity as

\[ u = \text{Fig. 4 Estimated errors vs. the number of BIA trials} \]

\[ \text{Fig. 5 Error-tolerance-adjusted BIA for the same case as in} \]

\[ \text{Fig. 4. The error tolerance adjustments occur at the 5th} \]

\[ \text{and 8th BIA trials. The vertical axis on the right is for the} \]

\[ \text{time accepted in green.} \]

\[ \text{3.2 Error-tolerance-adjusting scheme} \]

This problem was solved by the following tolerance adjusting scheme: It is usually the case that the estimated error rapidly decreases with decreasing time step size \( \Delta t \) for the first few BIA trials, irrespective of the errors being tolerable (accepted) or not. The dependence seems, by numerical investigation, to be

\[ \varepsilon \propto \Delta t^{-3}. \]

For the first few trials of the variable time step scheme explained above, estimated errors decrease rapidly. After such rapid decrement stage in estimated errors, the decrements become insensitive to the smaller time step \( \Delta t \) in some cases the estimated errors become larger for smaller time step size. Such an estimated error may be the attainable minimum error level by the BIA scheme. With this knowledge, the error tolerance is set twice the current one, when current estimated error is larger than one-fourth of the previous one, where one-fourth comes from the assumption that the estimated errors obey \( \varepsilon \propto \Delta t^2 \) for the rapid decreasing phase of the errors.

A test calculation with the error-tolerance-adjusting scheme is made for the same case presented in Fig. 3. Improvement against Fig. 4 is given in Fig. 5 and that for Fig. 3 in Fig. 6. In Fig. 4, the tolerance adjustments occur at the 5th and 8th BIA trials. In Fig. 6, the velocity at a time 100\( \Delta t \) given by the BIA with the error-tolerance-adjusting scheme is close to the by the DIM (Runge-Kutta-Fehlberg with an absolute error tolerance of \( 10^{-16} \)), as compared to that shown in Fig. 3. Thus the error-tolerance-adjusting scheme implemented into the BIA introduced in this study significantly improves the numerical accuracy of the BIA.

\[ \text{4. Summary} \]

Two accuracy assurance schemes are introduced to the Binary Interaction Approximation (BIA) to \( N \)-body problems. The first one is a sort of variable time step

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Since, in the framework of the BIA via Eq. (2), the relative force \( f_{ij}(t) \) changes the relative momentum \( \mu_{ij} g_{ij}(t) \),

\[
m_{i} \Delta v_{i} = \sum_{j \neq i}^{N} \mu_{ij} \left[ g_{ij}(t + \Delta t) - g_{ij}(t) \right]
\]

(A.3)

which is Eq. (4).

Similarly, the exact change \( \Delta r_{i} \) in position of the particle-\( i \) during \( \Delta t \) is formally given by

\[
\Delta r_{i} = \int_{t_{i}}^{t_{i} + \Delta t} v_{i}(t') \, dt'
= \int_{t_{i}}^{t_{i} + \Delta t} \left[ v_{i}(t) + \Delta v_{i}(t') \right] \, dt'
= \int_{t_{i}}^{t_{i} + \Delta t} \frac{d\xi}{dt'} \int_{t_{i}}^{t_{i}'} \frac{d\xi'}{dt''} \, dt''
\]

(A.4)

from which, with the BIA scheme, we have

\[
m_{i} \Delta r_{i} \approx m_{i} \rho_{i}(t) \Delta t + \int_{t_{i}}^{t_{i} + \Delta t} \frac{d\xi}{dt'} \int_{t_{i}}^{t_{i}'} \sum_{j \neq i}^{N} \mu_{ij} \frac{d\xi'}{dt''} \, dt''
= m_{i} \rho_{i}(t) \Delta t + \int_{t_{i}}^{t_{i} + \Delta t} \frac{d\xi}{dt'} \sum_{j \neq i}^{N} \mu_{ij} \left[ g_{ij}(t') - g_{ij}(t) \right]
= m_{i} \rho_{i}(t) \Delta t + \sum_{j \neq i}^{N} \mu_{ij} \left[ \Delta r_{ij} - g_{ij}(t) \Delta t \right],
\]

which is Eq. (3).