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ENERGY AND MOMENTUM CONSERVING METHODS OF ARBITRARY ORDER FOR THE NUMERICAL INTEGRATION OF EQUATIONS OF MOTION

II. Motion of a System of Particles

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ABSTRACT

In Part I of this work, numerical methods were derived for the solution of the equations of motion of a single particle subject to a central force which conserved exactly the energy and momenta. In the present work, the methodology of Part I is extended, in part, to motion of a system of particles, in that the energy and linear momentum are conserved exactly. In addition, the angular momentum will be conserved to one more order of accuracy than in conventional methods. Exact conservation of the total angular momentum results only for the lowest order numerical approximation, which is equivalent to the "discrete mechanics" presented elsewhere.

1. Introduction

The motion of a system of particles as determined from the laws of classical mechanics is widely used as a model in a variety of applications in physics. These applications range from statistical mechanics [1] and the interactions of atoms and molecules [2], to the motion of the solar system and space capsules [3] and the evolution of star clusters [4]. In each of these applications the conservation of the "additive constants of motion" -- the total energy, linear momentum, and angular momentum -- is of fundamental importance. Indeed, these conservation principles are the very essence of statistical mechanics [1].

Conventional numerical methods, when applied to the problem of the motion of a system of particles, do not lead to exact conservation of the total energy and momenta. The truncation error present in these methods disturbs the values of the constants of motion.

In previous work [5]-[8], a new numerical method -- "discrete mechanics" -- was developed, which exactly conserves the additive constants of motion. In [5], the basic conservative formulae were obtained for a separable, radially dependent potential of interaction ϕ. In [6], "discrete mechanics" was extended to include anisotropic potentials. Formulae for nonseparable ϕ were obtained in [7]. The theory was extended to an arbitrary numerical order of approximation for the case of the motion of a single particle in [8], Part I of this work. Part I also considered the questions of the truncation error and stability properties of the method, which were found to be the same as or superior to conventional techniques.

In the present work, the basic formulae presented in Part I are extended to the case of a system of particles. Unfortunately, except for the lowest-order approximation -- corresponding to the "discrete mechanics" presented previously [5] -- the new formulae conserve energy and linear momentum, but fail to conserve angular momentum. However, an extra order of numerical accuracy is obtained for this quantity.

The necessary mechanics of the motion of a system of particles is summarized in Sect. 2, the conventional numerical solutions reviewed in Sect. 3, and the conservative methods developed in Sects. 4 and 6. A numerical example is given in Sect. 5.

2. Equations of Motion

Suppose there are n particles, indexed by subscript i, subject to the influence of a potential of interaction ϕ. Let the mass of particle i be denoted by m_i and its position vector by $\vec{r}_i$,

$$\vec{r}_i = < X_i, Y_i, Z_i > \tag{2.1}$$

The velocity $\vec{v}_i$ of particle i is defined as the time derivative of $\vec{r}_i$:

$$\vec{v}_i = < \frac{dX_i}{dt}, \frac{dY_i}{dt}, \frac{dZ_i}{dt} > \tag{2.2}$$

If $\vec{r}_{ij}$ is the vector distance <u>from</u> particle i <u>to</u> particle j, then

$$\vec{r}_{ij} = \vec{r}_j - \vec{r}_i \tag{2.3a}$$

$$= < X_j - X_i, Y_j - Y_i, Z_j - Z_i > \tag{2.3b}$$

with corresponding time-derivative $\vec{v}_{ij}$ given by

$$\vec{v}_{ij} = \vec{v}_j - \vec{v}_i \tag{2.4}$$

Assume for simplicity that the potential ϕ is a pairwise-additive function of the distances r_{ij}:

$$\phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n) = \phi_{12}(r_{12}) + \phi_{13}(r_{13}) + \ldots + \phi_{n-1,n}(r_{n-1,n}) \tag{2.5a}$$

$$= \sum_{i<j} \phi_{ij}(r_{ij}) \tag{2.5b}$$

where

$$r_{ij} \equiv |\vec{r}_{ij}| \equiv [(X_j - X_i)^2 + (Y_j - Y_i)^2 + (Z_j - Z_i)^2]^{1/2} \qquad (2.6)$$

and

$$\sum_{i<j} \equiv \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \equiv \sum_{j=2}^{n} \sum_{i=1}^{j-1} \qquad (2.7)$$

Note since, by eq. (2.3a),

$$\vec{r}_{ji} = -\vec{r}_{ij} \qquad (2.8)$$

then by eqs. (2.6)

$$r_{ji} = r_{ij} \qquad (2.9)$$

Many fundamental physical interactions have potentials of the form given by eq. (2.5b). For example, gravitational forces are characterized by

$$\phi_{ij}(r_{ij}) = -\frac{G\, m_i\, m_j}{r_{ij}} \qquad (2.10)$$

where G is the gravitational constant. On the other hand, certain potentials corresponding to molecular interactions (with averaged electronic motions) do not have the additive form of eqs. (2.5). The generalization of the results of Sect. 4 to more complicated ϕ is mentioned in Sect. 7.

Newton's equations of motion for the system of particles are

$$m_i \vec{a}_i = \vec{F}_i \qquad (i=1,2,\ldots,n) \tag{2.11}$$

where

$$\vec{a}_i = \frac{d^2\vec{r}_i}{dt^2} \tag{2.12}$$

is the acceleration of particle i; $\vec{F}_i$ is the force on i due to the action of the potential ϕ, given by

$$\vec{F}_i = -\frac{\partial\phi}{\partial\vec{r}_i} \tag{2.13}$$

where

$$\frac{\partial}{\partial\vec{r}_i} = \left\langle \frac{\partial}{\partial X_i}, \frac{\partial}{\partial Y_i}, \frac{\partial}{\partial Z_i} \right\rangle \tag{2.14}$$

is the gradient with respect to $\vec{r}_i$. Using the chain-rule and eqs. (2.3), (2.5) and (2.13),

$$\vec{F}_i = -\sum_{j=1}^{i-1} \frac{d\phi_{ji}}{dr_{ji}} \frac{\partial r_{ji}}{\partial\vec{r}_i} - \sum_{j=i+1}^{n} \frac{d\phi_{ij}}{dr_{ij}} \frac{\partial r_{ij}}{\partial\vec{r}_i} \tag{2.15a}$$

$$= -\sum_{j=1}^{i-1} \frac{d\phi_{ji}}{dr_{ji}} \frac{\partial r_{ji}}{\partial\vec{r}_{ji}} \frac{\partial\vec{r}_{ji}}{\partial\vec{r}_i} - \sum_{j=i+1}^{n} \frac{d\phi_{ij}}{dr_{ij}} \frac{\partial r_{ij}}{\partial\vec{r}_{ij}} \frac{\partial\vec{r}_{ij}}{\partial\vec{r}_i} \tag{2.15b}$$

$$= -\sum_{j=1}^{i-1} \frac{d\phi_{ji}}{dr_{ji}} \frac{\vec{r}_{ji}}{r_{ji}} + \sum_{j=i+1}^{n} \frac{d\phi_{ij}}{dr_{ij}} \frac{\vec{r}_{ij}}{r_{ij}} \tag{2.15c}$$

Defining

$$\vec{F}_{ij} = - \frac{\partial \phi_{ij}}{\partial \vec{r}_{ij}} \qquad (i<j) \tag{2.16a}$$

$$= - \frac{d\phi_{ij}}{dr_{ij}} \frac{\vec{r}_{ij}}{r_{ij}} \tag{2.16b}$$

and

$$\vec{F}_{ji} = \begin{cases} -\vec{F}_{ij} & (i<j) \\ 0 & (i=j) \end{cases} \tag{2.17}$$

then eqs. (2.15) can be written

$$\vec{F}_i = - \sum_{j=1}^{n} \vec{F}_{ij} \qquad (i=1,2,\ldots n) \tag{2.18}$$

so that the equations of motion (2.11) become

$$m_i \frac{d^2\vec{r}_i}{dt^2} = - \sum_{j=1}^{n} \vec{F}_{ij} \qquad (i=1,2,\ldots n) \tag{2.19}$$

It will be of interest for later consideration to examine the quantity $\vec{a}_{ij}$, defined by

$$\vec{a}_{ij} = \frac{d\vec{v}_{ij}}{dt} \tag{2.20a}$$

$$= \vec{a}_j - \vec{a}_i \tag{2.20b}$$

Substitution of eq. (2.19) for the $\vec{a}_i$ then yields

$$\vec{a}_{ij} = \sum_{k=1}^{n} \left(\frac{\vec{F}_{kj}}{m_j} - \frac{\vec{F}_{ki}}{m_i}\right) \tag{2.21}$$

The total angular momentum $\vec{L}$ of the system of particles is given by

$$\vec{L} = \sum_{i=1}^{n} m_i(\vec{r}_i \times \vec{v}_i) \tag{2.22}$$

where $\vec{r}_i \times \vec{v}_i$ denotes the vector cross product with components

$$\vec{r}_i \times \vec{v}_i = \left< Y\frac{dZ}{dt} - Z\frac{dY}{dt},\ Z\frac{dX}{dt} - X\frac{dZ}{dt},\ X\frac{dY}{dt} - Y\frac{dX}{dt} \right> \tag{2.23}$$

Conservation of angular momentum is expressed by the equation

$$\frac{d\vec{L}}{dt} = 0 \tag{2.24}$$

so that, for any two times t and t',

$$\vec{L}(t') = \vec{L}(t) \tag{2.25}$$

where $\vec{L}$ is evaluated along the trajectory. Verification of eq. (2.24) is easily obtained by noting that

$$\frac{d\vec{L}}{dt} = \sum_{i=1}^{n} m_i \frac{d}{dt}(\vec{r}_i \times \vec{v}_i) \tag{2.26a}$$

$$= \sum_{i=1}^{n} m_i(\vec{r}_i \times \vec{a}_i) \tag{2.26b}$$

$$= \sum_{i=1}^{n} \vec{r}_i \times \vec{F}_i \tag{2.26c}$$

Substitution of eq. (2.18) into (2.26) then gives

$$\frac{d\vec{L}}{dt} = - \sum_{i=1}^{n} \sum_{j=1}^{n} \vec{r}_i \times \vec{F}_{ij} \tag{2.27a}$$

$$= - \sum_{i<j} \vec{r}_i \times \vec{F}_{ij} - \sum_{j<i} \vec{r}_i \times \vec{F}_{ij} \tag{2.27b}$$

$$= \sum_{i<j} \vec{r}_{ij} \times \vec{F}_{ij} \tag{2.27c}$$

Since the vector direction of $\vec{F}_{ij}$ is $\vec{r}_{ij}$ from eq. (2.16), each of the terms $\vec{r}_{ij} \times \vec{F}_{ij}$ vanishes, and eq. (2.24) is obtained. Note that conservation of angular momentum is obtained independently of the functional forms of the ϕ_{ij}.

The total energy E is given by

$$E = \sum_{i=1}^{n} \frac{1}{2} m_i(\vec{v}_i \cdot \vec{v}_i) + \phi \tag{2.28}$$

where $\vec{\alpha} \cdot \vec{\beta}$ denotes the scalar product of two vectors $\vec{\alpha}$ and $\vec{\beta}$. Conservation of E is expressed by

$$\frac{dE}{dt} = 0 \tag{2.29}$$

or

$$E(t') = E(t)$$

for any two times t and t' along the trajectory.

With regard to conservation of total linear momentum, (and consequently the center of mass motion), the only requirement is consistency, which is a property of the pairwise-additive formulation and therefore, interestingly enough, of every numerical method of order 2 or higher. For this reason, conservation of total linear momentum will not receive special attention.

3. Conventional Numerical Solutions

Three commonly used methods for the numerical solution of the differential eqs. (2.19) are the truncated Taylor-series, Runge-Kutta, and Adams' predictor-corrector formulae. In each of these methods, the $\vec{r}_i(t)$ and $\vec{v}_i(t)$ and previous values of the forces or derivatives of the forces are used to construct the calculated values $\vec{r}'_{c,i}$ and $\vec{v}'_{c,i}$ for

$$\vec{r}'_i = \vec{r}_i(t') \tag{3.1a}$$

$$\vec{v}'_i = \vec{v}_i(t') \tag{3.1b}$$

at the new time $t' = t + \Delta t$.

The truncated Taylor-series and Adams' formulae will now be reviewed in order to allow a comparison with the new methods to be developed in Sect. 4.

A. Taylor-Series Method

For a sufficiently small time step Δt, the $\vec{r}'_i$ and $\vec{v}'_i$ may be obtained via the Taylor-series formulae

$$\vec{r}'_i = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n}{}' \left[\vec{F}_{ji} \frac{(\Delta t)^2}{2!} + \vec{G}_{ji} \frac{(\Delta t)^3}{3!} + \ldots\right] \tag{3.2a}$$

$$\vec{v}'_i = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n}{}' \left[\vec{F}_{ji} \frac{\Delta t}{1!} + \vec{G}_{ji} \frac{(\Delta t)^2}{2!} + \ldots\right] \tag{3.2b}$$

obtained via eqs. (2.19), and where

$$\vec{G}_{ji} = \frac{d\,\vec{F}_{ji}}{dt} \tag{3.3}$$

etc. The explicit form of the $\vec{G}_{ji}$ may be obtained by noting that no explicit time dependence occurs in eqs. (2.19), and thus, by the chain-rule, and (2.21)

$$\frac{d}{dt} = \sum_{k<\ell} \left[\frac{d\vec{r}_{k\ell}}{dt} \cdot \frac{\partial}{\partial r_{k\ell}} + \frac{d\vec{v}_{k\ell}}{dt} \cdot \frac{\partial}{\partial \vec{v}_{k\ell}} \right] \tag{3.4a}$$

$$= \sum_{k<\ell} \left[\vec{v}_{k\ell} \cdot \frac{\partial}{\partial \vec{r}_{k\ell}} + \vec{a}_{k\ell} \cdot \frac{\partial}{\partial \vec{v}_{k\ell}} \right] \tag{3.4b}$$

$$= \sum_{k<\ell} \left[\vec{v}_{k\ell} \cdot \frac{\partial}{\partial \vec{r}_{k\ell}} + \sum_{p=1}^{n} \left(\frac{\vec{F}_{p\ell}}{m_\ell} - \frac{\vec{F}_{pk}}{m_k} \right) \cdot \frac{\partial}{\partial \vec{v}_{k\ell}} \right] \tag{3.4c}$$

where, as before, $\vec{\alpha} \cdot \vec{\beta}$ denotes the scalar product of $\vec{\alpha}$ and $\vec{\beta}$. Relation (3.4) allows successive time differentiations of eqs. (2.19) recursively. In the case of $\vec{G}_{ij}$, the $\vec{F}_{ij}$ are given in the form

$$\vec{F}_{ij} = f_{ij}\,\vec{r}_{ij} \tag{3.5}$$

where

$$f_{ij} = -\frac{1}{r_{ij}} \frac{d\phi_{ij}}{dr_{ij}} \tag{3.6}$$

from eq. (2.16). Therefore, via eqs. (3.3) and (3.4),

$$\vec{G}_{ij} = \frac{df_{ij}}{dr_{ij}}\,\dot{r}_{ij}\,\vec{r}_{ij} + f_{ij}\,\vec{v}_{ij} \tag{3.7}$$

where

$$\dot{r}_{ij} = \frac{dr_{ij}}{dt} \tag{3.8a}$$

$$= \frac{1}{r_{ij}} (\vec{r}_{ij} \cdot \vec{v}_{ij}) \tag{3.8b}$$

is the radial component of the velocity, and (via eq. (3.6))

$$\frac{df_{ij}}{dr_{ij}} = - \frac{1}{r_{ij}} [f_{ij} + \frac{d^2 \phi_{ij}}{dr_{ij}^2}] \tag{3.9}$$

From eq. (3.7b), it can be seen that $\vec{G}_{ij}$ has components only in the two directions $\vec{r}_{ij}$ and $\vec{v}_{ij}$.

The calculated values $\vec{r}'_{c,i}$ and $\vec{v}'_{c,i}$ are usually obtained by truncating eqs. (3.2) at some point. For example, stopping at the $\vec{F}_{ij}$ terms gives

$$\vec{r}'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} \vec{F}_{ji} \frac{(\Delta t)^2}{2} \tag{3.10a}$$

$$\vec{v}'_{c,i} = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} \vec{F}_{ji} (\Delta t) \tag{3.10b}$$

so that the "truncation errors" are given by

$$\vec{r}'_i = \vec{r}'_{c,i} + O[(\Delta t)^3] \tag{3.11a}$$

$$\vec{v}'_i = \vec{v}'_{c,i} + O[(\Delta t)^2] \tag{3.11b}$$

Higher-order approximations are simply obtained by including more terms in eqs. (3.2). For example, stopping at the $\vec{G}_{ij}$ gives

$$\vec{r}\,'_{c,i} = \vec{r}_i + \vec{v}_i\,\Delta t + \frac{1}{m_i}\sum_{j=1}^{n}\left[\vec{F}_{ji}\frac{(\Delta t)^2}{2} + \vec{G}_{ji}\frac{(\Delta t)^3}{6}\right] \tag{3.12a}$$

$$\vec{v}\,'_{c,i} = \vec{v}_i + \frac{1}{m_i}\sum_{j=1}^{n}\left[\vec{F}_{ji}\,\Delta t + \vec{G}_{ji}\frac{(\Delta t)^2}{2}\right] \tag{3.12b}$$

so that

$$\vec{r}\,'_i = \vec{r}\,'_{c,i} + O[(\Delta t)^4] \tag{3.13a}$$

$$\vec{v}\,'_i = \vec{v}\,'_{c,i} + O[(\Delta t)^3] \tag{3.13b}$$

In each of these Taylor-series methods, the truncation errors in the $\vec{r}\,'_{c,i}$ and $\vec{v}\,'_{c,i}$ lead to corresponding errors in $\vec{L}$ and E, so that these quantities are no longer exactly conserved. It is instructive to observe the mechanism by which the error in, e.g., $\vec{L}$ is introduced. The lack of conservation in $\vec{L}$ over the time-step Δt is given by the quantity $\Delta\vec{L}_c$ defined by

$$\Delta\vec{L}_c = \vec{L}'_c - \vec{L} \tag{3.14a}$$

$$= \sum_{i=1}^{n} m_i[\vec{r}\,'_{c,i}\times\vec{v}\,'_{c,i} - \vec{r}_i\times\vec{v}_i] \tag{3.14b}$$

For the case of the simple method of eqs. (3.10),

$$m_i\,\vec{r}\,'_{c,i}\times\vec{v}\,'_{c,i} = m_i\,\vec{r}_i\times\vec{v}_i + \sum_{j=1}^{n}\left[\vec{r}_i\times\vec{F}_{ji}\,\Delta t + \vec{v}_i\times\vec{F}_{ji}\frac{(\Delta t)^2}{2}\right] \tag{3.15}$$

Substitution of this result into eqs. (3.14) now gives

$$\Delta\vec{L}_c = \sum_{i=1}^{n} \sum_{j=1}^{n} [\vec{r}_i \times \vec{F}_{ji} \Delta t + \vec{v}_i \times \vec{F}_{ji} \frac{(\Delta t)^2}{2}] \tag{3.16a}$$

$$= \sum_{i<j} [\vec{r}_i \times \vec{F}_{ji} \Delta t + \vec{v}_i \times \vec{F}_{ji} \frac{(\Delta t)^2}{2}]$$

$$+ \sum_{j<i} [\vec{r}_i \times \vec{F}_{ji} \Delta t + \vec{v}_i \times \vec{F}_{ji} \frac{(\Delta t)^2}{2}] \tag{3.16b}$$

$$= - \sum_{i<j} [\vec{r}_i \times \vec{F}_{ij} \Delta t + \vec{v}_i \times \vec{F}_{ij} \frac{(\Delta t)^2}{2}]$$

$$+ \sum_{i<j} [\vec{r}_j \times \vec{F}_{ij} \Delta t + \vec{v}_j \times \vec{F}_{ij} \frac{(\Delta t)^2}{2}] \tag{3.16c}$$

$$= \sum_{i<j} [\vec{r}_{ij} \times \vec{F}_{ij} \Delta t + \vec{v}_{ij} \times \vec{F}_{ij} \frac{(\Delta t)^2}{2}] \tag{3.16d}$$

Since by eq. (3.5) $\vec{F}_{ij}$ lies along $\vec{r}_{ij}$, the first term in eq. (3.16d) vanishes leaving

$$\Delta\vec{L}_c = \frac{(\Delta t)^2}{2} \sum_{i<j} \vec{v}_{ij} \times \vec{F}_{ij} \tag{3.17a}$$

$$= \frac{(\Delta t)^2}{2} \sum_{i<j} f_{ij} \vec{v}_{ij} \times \vec{r}_{ij} \tag{3.17b}$$

$$= O[(\Delta t)^2] \tag{3.17c}$$

As expected, there is a lack of conservation of $\vec{L}$ of $O[(\Delta t)^2]$ corresponding to the truncation error in $\vec{v}'_{c,i}$.

For the case of the third-order method of eqs. (3.12), it follows, as above, that

$$\Delta\vec{L}_c = \sum_{i<j} [\vec{r}_{ij} \times \vec{F}_{ij} \Delta t + \frac{(\Delta t)^2}{2} (\vec{v}_{ij} \times \vec{F}_{ij} + \vec{r}_{ij} \times \vec{G}_{ij}) + \frac{(\Delta t)^3}{3} \vec{v}_{ij} \times \vec{G}_{ij} + \frac{(\Delta t)^4}{12} \vec{a}_{ij} \times \vec{G}_{ij}] \quad (3.18)$$

where eq. (2.21) has been used. The first term in eq. (3.18) vanishes because of eq. (3.5). Now consider the $(\Delta t)^2$ term in eq. (3.18). Substitution of eqs. (3.5) and (3.7) give

$$\vec{v}_{ij} \times \vec{F}_{ij} + \vec{r}_{ij} \times \vec{G}_{ij} = f_{ij} \vec{v}_{ij} \times \vec{r}_{ij} + f_{ij} \vec{r}_{ij} \times \vec{v}_{ij} + \frac{df_{ij}}{dr_{ij}} \dot{r}_{ij} \vec{r}_{ij} \times \vec{r}_{ij} \quad (3.19a)$$

$$= f_{ij} \vec{v}_{ij} \times \vec{r}_{ij} + f_{ij} \vec{r}_{ij} \times \vec{v}_{ij} \quad (3.19b)$$

$$= \vec{0} \quad (3.19c)$$

so that

$$\Delta\vec{L}_c = \frac{(\Delta t)^3}{3} \sum_{i<j} \vec{v}_{ij} \times \vec{G}_{ij} + O[(\Delta t)^4] \quad (3.20a)$$

$$= \frac{(\Delta t)^3}{3} \sum_{i<j} \frac{df_{ij}}{dr_{ij}} \dot{r}_{ij} \vec{v}_{ij} \times \vec{r}_{ij} + O[(\Delta t)^4] \quad (3.20b)$$

or, finally,

$$\Delta\vec{L}_c = O[(\Delta t)^3] \quad (3.21)$$

Again, as expected, the lack of conservation of $\vec{L}$ is of the same order as the truncation error in $\vec{v}'_{c,i}$.

In general the truncation errors of the $\vec{v}'_{c,i}$ lead to errors of the same orders in $\vec{L}$ and E, and exact conservation of either quantity only occurs in the limit $\Delta t \to 0$.

B. Adams' Method

The essence of the Adams' methods is to interpolate the derivatives in eqs. (3.2) by using values of the $\vec{F}_{ij}$ over several time steps. The lowest order Adams' attempts to approximate $\vec{G}_{ij}$ by the formula

$$\vec{G}_{ij} = [(\vec{F}'_{c,ij} - \vec{F}_{ij})/\Delta t] + O(\Delta t) \quad (3.22)$$

where

$$\vec{F}'_{c,ij} = \vec{F}_{ij}(\vec{r}'_{c,ij}) \quad (3.23)$$

Eqs. (3.22) and (3.23) gives rise to the Adams' formulae

$$\vec{r}\,'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{(\Delta t)^2}{3m_i} \sum_{j=1}^{n} [\vec{F}_{ij} + \frac{1}{2} \vec{F}\,'_{c,ij}] \qquad (3.24a)$$

$$\vec{v}\,'_{c,i} = \vec{v}_i + \frac{\Delta t}{2m_i} \sum_{j=1}^{n} [\vec{F}_{ij} + \vec{F}\,'_{c,ij}] \qquad (3.24b)$$

$$\vec{F}\,'_{c,ij} = \vec{F}_{ij}(\vec{r}\,'_{c,ij}) \qquad (3.24c)$$

Higher-order formulae are obtained by multipoint approximations to the derivatives using values of the $\vec{F}_{ij}$ at times $t - \Delta t$, $t - 2\Delta t$, etc.

Eqs. (3.24) are implicit in the $\vec{r}\,'_{c,i}$ via the $\vec{F}\,'_{c,ij}$. For small enough Δt, the equations may be solved by starting with

$$\vec{F}\,'_{c,ij} \simeq \vec{F}_{ij} \qquad (3.25)$$

and iteratively finding the $\vec{r}\,'_{c,ij}$ and reevaluating the $\vec{F}\,'_{c,ij}$. Since eq. (3.22) holds,

$$\vec{r}\,'_i = \vec{r}\,'_{c,i} + O[(\Delta t)^4] \qquad (3.26a)$$

$$\vec{r}\,'_i = \vec{v}\,'_{c,i} + O[(\Delta t)^3] \qquad (3.26b)$$

and

$$\Delta\vec{L}_c = O[(\Delta t)^3] \qquad (3.27)$$

similar to the third-order Taylor-series method of Sect. 3.A above.

4. Maximally Conservative Solutions

The Taylor-series and Adams' methods of Sect. 3 suffer the defect of not preserving the total energy and angular momentum at their initial values: these quantities are disturbed by the presence of the truncation errors in the $\vec{r}'_{c,i}$ and $\vec{v}'_{c,i}$. Since any numerical method which conserves the constants of motion is necessarily that much more strongly linked to the correct solution, this is a very desirable feature to build into an approximate solution.

In Part I [8], a conservation method of arbitrary order of accuracy was found for the case of a single particle subject to a central force (or two interacting particles). In what follows an attempt is made to extend that result to a system of particles. As in Part I, two formulations are given, explicit and implicit in the $\vec{r}'_{c,i}$. Although conservation of energy will be obtained in all cases, the total angular momentum is conserved, in general, only to one more order of accuracy than in the corresponding conventional methods. Exact conservation of $\vec{L}$ is obtained, however, for the lowest-order method, and in the case of a single interaction.

The method used to obtain the maximally conservative formulae is to construct the quantities $\Delta\vec{L}_c$ and ΔE_c, transform to the $i < j$ forms, and solve for zero contributions as far as possible. The lowest-order formulae, corresponding to the second- and third-order methods of Sect. 3 will be used throughout the derivation, although the results easily extend to higher orders of accuracy in Δt. Indeed, in Sect. 6, we will, for completeness, outline the formulae for the explicit and implicit methods of arbitrary order, for the case of a Taylor-series type method.

A. Explicit Formulation

i. Second-Order Method

Consider first the simple formulae

$$\vec{r}\,'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} \vec{F}_{ji} \frac{(\Delta t)^2}{2} \tag{4.1a}$$

$$\vec{v}\,'_{c,i} = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} \vec{F}^*_{ji} \Delta t \tag{4.1b}$$

where the $\vec{F}_{ji}$ in eq. (3.10b) have been replaced by the arbitrary quantities $\vec{F}^*_{ji}$. What is desired is to find values for the $\vec{F}^*_{ji}$ such that $\vec{F}^*_{ij} = -\vec{F}^*_{ji}$ and

$$\vec{F}^*_{ji} = \vec{F}_{ji} + O[\Delta t] \tag{4.2}$$

and so that $\vec{L}$ and E are maximally conserved. Constructing $\Delta\vec{L}_c$,

$$\Delta\vec{L}_c = \sum_{i=1}^{n} m_i[\vec{r}'_{c,i} \times \vec{v}'_{c,i} - \vec{r}_i \times \vec{v}_i] \tag{4.3a}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} [\vec{F}_{ji} \times \vec{v}_i \frac{(\Delta t)^2}{2} + \vec{r}'_{c,i} \times \vec{F}^*_{ji} \Delta t] \tag{4.3b}$$

$$= \Delta t \sum_{i<j}^{n} [\vec{F}_{ij} \times \vec{v}_{ij} \frac{\Delta t}{2} + \vec{r}'_{c,ij} \times \vec{F}^*_{ij}] \tag{4.3c}$$

where

$$\vec{r}'_{c,ij} = \vec{r}'_{c,j} - \vec{r}'_{c,i} \tag{4.4a}$$

$$= \vec{r}_{ij} + \vec{v}_{ij} \Delta t + \vec{a}_{ij} \frac{(\Delta t)^2}{2} \tag{4.4b}$$

Clearly the choice $\vec{F}^*_{ij} = \vec{F}_{ij}$ results in the method of eq. (3.10), with $\Delta\vec{L}_c = O[(\Delta t)^2]$ from eq. (3.17). Maximal conservation of $\vec{L}$ results if the $\vec{F}^*_{ij}$ are chosen so that each term in eq. (4.3) is as close to zero as possible. Setting

$$\vec{r}'_{c,ij} \times [\vec{F}_{ij} \times \vec{v}_{ij} \frac{\Delta t}{2} + \vec{r}'_{c,ij} \times \vec{F}^*_{ij}] = \vec{0} \tag{4.5}$$

(which is the best that can be done) results in

$$\vec{F}^*_{ij} = \epsilon_{ij} \vec{r}'_{c,ij} + \vec{\beta}_{ij} \frac{\Delta t}{2} \tag{4.6}$$

where

$$\epsilon_{ij} = \frac{\vec{r}'_{c,ij} \cdot \vec{F}^*_{ij}}{(r'_{c,ij})^2} \tag{4.7}$$

is the (unknown) component of $\vec{F}^*_{ij}$ in direction $\vec{r}'_{c,ij}$, and

$$\vec{\beta}_{ij} = \frac{1}{(r'_{c,ij})^2} [(\vec{r}'_{c,ij} \cdot \vec{v}_{ij}) \vec{F}_{ij} - (\vec{r}'_{c,ij} \cdot \vec{F}_{ij})\vec{v}_{ij}] \qquad (4.8)$$

At this point, it is opportune to examine the error $\Delta\vec{L}_c$ made through the use of formula (4.6) for the $\vec{F}^*_{ij}$. From eq. (4.3c), with substitution of eq. (4.6),

$$\Delta\vec{L}_c = \Delta t \sum_{i<j} [\vec{F}_{ij} \times \vec{v}_{ij} \frac{\Delta t}{2} + \vec{r}'_{c,ij} \times \vec{\beta}_{ij} \frac{\Delta t}{2}] \qquad (4.9a)$$

$$= \frac{(\Delta t)^2}{2} \sum_{i<j} [\vec{F}_{ij} \times \vec{v}_{ij} + \frac{\vec{r}'_{c,ij} \cdot \vec{F}_{ij} \times \vec{v}_{ij}}{(r'_{c,ij})^2} \vec{r}'_{c,ij} - \vec{F}_{ij} \times \vec{v}_{ij}] \qquad (4.9b)$$

$$= \frac{(\Delta t)^2}{2} \sum_{i<j} \frac{[\vec{r}'_{c,ij} \cdot \vec{F}_{ij} \times \vec{v}_{ij}]}{(r'_{c,ij})^2} \vec{r}'_{c,ij} \qquad (4.9c)$$

The scalar triple product $\vec{a}\cdot\vec{b}\times\vec{c}$ of three vectors vanishes if $\vec{a}$, $\vec{b}$, and $\vec{c}$ are coplanar. Noting that $\vec{F}_{ij}$ lies along direction $\vec{r}_{ij}$, via eq. (4.1),

$$\vec{r}'_{c,ij} = \vec{r}_{ij} + \vec{v}_{ij} \Delta t + \vec{a}_{ij} \frac{(\Delta t)^2}{2} \qquad (4.10)$$

then

$$\Delta\vec{L}_c = \frac{(\Delta t)^4}{4} \sum_{i<j} \frac{[\vec{a}_{ij} \cdot \vec{F}_{ij} \times \vec{v}_{ij}]}{(r'_{c,ij})^2} \vec{r}'_{c,ij} \tag{4.11a}$$

$$= \frac{(\Delta t)^4}{4} \sum_{i<j} \frac{\vec{r}'_{c,ij}}{(r'_{c,ij})^2} \sum_{k \neq i,j} \left(\frac{\vec{F}_{kj}}{m_j} - \frac{\vec{F}_{ki}}{m_i}\right) \cdot \vec{F}_{ij} \times \vec{v}_{ij} \tag{4.11b}$$

$$= O[(\Delta t)^4] \tag{4.11c}$$

which is to be compared with the error of $O[(\Delta t)^2]$ which resulted from the choice $\vec{F}^*_{ij} = \vec{F}_{ij}$ in eq. (3.10b). Note that in the special case of only two particles $(n = 2)$, the sum over k in eq. (4.11b) is empty, and $\vec{L}$ is exactly conserved, agreeing with the results of [8].

Formula (4.6) for the $\vec{F}^*_{ij}$ is incomplete because the ϵ_{ij} are yet to be determined. Using eq. (2.28), the error ΔE_c made in the energy over the time step Δt is

$$\Delta E_c = \frac{1}{2} \sum_{i=1}^{n} m_i [\vec{v}'_{c,i} \cdot \vec{v}'_{c,i} - \vec{v}_i \cdot \vec{v}_i] + \Delta\phi \tag{4.12}$$

where

$$\Delta\phi = \sum_{i<j} [\phi'_{c,ij} - \phi_{ij}] \tag{4.13}$$

and

$$\phi'_{c,ij} = \phi_{ij}(r'_{c,ij}) \tag{4.14}$$

Substitution of formula (4.1b) for the $\vec{v}'_{c,i}$ into eq. (4.12) gives

$$\Delta E_c = \frac{1}{2} \sum_{i=1}^{n} m_i [\vec{v}_i \cdot \vec{v}_i + \frac{2\Delta t}{m_i} \sum_{j=1}^{n} \vec{v}_i \cdot \vec{F}^*_{ji}$$

$$+ \frac{(\Delta t)^2}{m_i^2} \sum_{j=1}^{n} \sum_{k=1}^{n} \vec{F}^*_{ki} \cdot \vec{F}^*_{ji} - \vec{v}_i \cdot \vec{v}_i] + \Delta\phi \quad (4.15a)$$

$$= \Delta t \sum_{i=1}^{n} \sum_{j=1}^{n} [\vec{v}_i \cdot \vec{F}^*_{ji} + \frac{\Delta t}{2m_i} \sum_{k=1}^{n} \vec{F}^*_{ki} \cdot \vec{F}^*_{ji}] + \Delta\phi \quad (4.15b)$$

Transforming to the $i < j$ form,

$$\Delta E_c = -\Delta t \sum_{i<j} [\vec{v}_i \cdot \vec{F}^*_{ij} + \frac{\Delta t}{2m_i} \sum_{k=1}^{n} \vec{F}^*_{ki} \cdot \vec{F}^*_{ij}]$$

$$+ \Delta t \sum_{j<i} [\vec{v}_i \cdot \vec{F}^*_{ji} + \frac{\Delta t}{2m_i} \sum_{k=1}^{n} \vec{F}^*_{ki} \cdot \vec{F}^*_{ji}] + \Delta\phi \quad (4.16a)$$

$$= \Delta t \sum_{i<j} [\vec{v}_{ij} \cdot \vec{F}^*_{ij} + \frac{\Delta t}{2} \sum_{k=1}^{n} (\frac{\vec{F}^*_{kj}}{m_j} - \frac{\vec{F}^*_{ki}}{m_i}) \cdot \vec{F}^*_{ij}] + \Delta\phi \quad (4.16b)$$

$$= \Delta t \sum_{i<j} [(\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2}) \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}] \quad (4.16c)$$

where

$$\vec{a}^*_{ij} = \sum_{k=1}^{n} (\frac{\vec{F}^*_{kj}}{m_j} - \frac{\vec{F}^*_{ki}}{m_i}) \quad (4.17)$$

and

$$\Delta\phi_{ij} = \phi'_{c,ij} - \phi_{ij} \tag{4.18}$$

In order to make ΔE_c vanish it suffices to choose the set of ϵ_{ij} such that

$$(\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2}) \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t} = 0 \tag{4.19}$$

Since each of $\vec{F}^*_{ij}$, $\vec{v}'_{c,ij}$, and $\vec{a}^*_{ij}$ are linearly dependent on the ϵ_{ij}, eqs. (4.19) represent a quadratic system of equations for the ϵ_{ij}. A first approximation for ϵ_{ij} may be obtained by noting that

$$\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2} = \vec{v}_{ij} + O[\Delta t] \tag{4.20}$$

so that for the correct root

$$\vec{v}_{ij} \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t} = O[\Delta t] \tag{4.21}$$

Substituting eq. (4.6) for the $\vec{F}^*_{ij}$,

$$(\vec{v}_{ij} \cdot \vec{r}'_{c,ij})\epsilon_{ij} + (\vec{v}_{ij} \cdot \vec{\beta}_{ij}) \frac{\Delta t}{2} + \frac{\Delta\phi_{ij}}{\Delta t} = O[\Delta t] \tag{4.22}$$

which implies

$$\epsilon_{ij} = - \frac{\Delta\phi_{ij}}{(\vec{r}_{ij} \cdot \vec{v}_{ij})\Delta t} + O[\Delta t] \tag{4.23}$$

Since $\phi_{ij} = \phi_{ij}(r_{ij})$, it follows from eqs. (3.6), and (3.8b) that

$$\phi_{ij}(r'_{c,ij}) = \phi_{ij}(r_{ij}) + \frac{d\phi_{ij}}{dr_{ij}} (r'_{c,ij} - r_{ij}) + O[(\Delta t)^2] \tag{4.24a}$$

$$= \phi_{ij} - f_{ij}(\vec{r}_{ij} \cdot \vec{v}_{ij})\Delta t + O[(\Delta t)^2] \tag{4.24b}$$

where

$$r'_{c,ij} = r_{ij} + \dot{r}_{ij} \Delta t + O[(\Delta t)^2] \tag{4.25}$$

Substitution of eq. (4.24b) into eq. (4.23) now gives

$$\epsilon_{ij} = f_{ij} + O[\Delta t] \tag{4.26}$$

which gives

$$\vec{F}^*_{ij} = f_{ij} \vec{r}'_{c,ij} + O[\Delta t] \tag{4.27a}$$

$$= f_{ij} \vec{r}_{ij} + O[\Delta t] \tag{4.27b}$$

$$= \vec{F}_{ij} + O[\Delta t] \tag{4.27c}$$

as expected. (Compare eq. (4.2)).

Since eq. (4.23) holds for small Δt, in this case eqs. (4.19) are strongly linear (the nonlinear terms are one order higher in Δt), and can be solved iteratively. For example, noting that

$$\frac{\partial \vec{a}^*_{ij}}{\partial \epsilon_{ij}} = \left(\frac{1}{m_i} + \frac{1}{m_j}\right) \frac{\partial \vec{F}^*_{ij}}{\partial \epsilon_{ij}} \tag{4.28}$$

and

$$\frac{\partial \vec{F}^*_{ij}}{\partial \epsilon_{ij}} = \vec{r}\,'_{c,ij} \tag{4.29}$$

the Newton iteration for each ϵ_{ij} independently is given by

$$\epsilon^{(k+1)}_{ij} = \epsilon^{(k)}_{ij} - \left. \frac{(\vec{v}_{ij} + \vec{a}^*_{ij}\frac{\Delta t}{2}) \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}}{\vec{r}\,'_{c,ij} \cdot [\vec{v}_{ij} + \vec{a}^*_{ij}\frac{\Delta t}{2} + \frac{\Delta t}{2}(\frac{1}{m_i} + \frac{1}{m_j})\vec{F}^*_{ij}]} \right|_k \tag{4.30}$$

where k is the iteration number, $\epsilon^{(k)}_{ij}$ is the k-th approximation to ϵ_{ij}, and $|_k$ denotes evaluation using the $\epsilon^{(k)}_{ij}$. Eq. (4.30) must be iterated to convergence in order that eq. (4.19) be satisfied and the energy exactly conserved.

As long as $\dot{r}_{ij}$ is of order of unity, eq. (4.23) holds and the iteration eq. (4.30) is self-starting. In this case the starting values

$$\epsilon_{ij}^{(0)} = 0 \tag{4.31}$$

are convenient. In the event $\dot{r}_{ij} = O[\Delta t]$, the starting values

$$\epsilon_{ij}^{(0)} = f_{ij} \tag{4.32}$$

or the ϵ_{ij} from the previous step are appropriate.

ii. Third-Order Method

An extension of the formulae of Section 4.A.i. to higher-order methods is now obvious. E.g., consider the third-order formulae of eqs. (3.12) with the $\vec{G}_{ji}$ in eq. (3.12b) replaced with $\vec{G}^*_{ji}$:

$$\vec{r}'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} [\vec{F}_{ji} \frac{(\Delta t)^2}{2} + \vec{G}_{ji} \frac{(\Delta t)^3}{6}] \tag{4.33a}$$

$$\vec{v}'_{c,i} = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} [\vec{F}_{ji} \frac{(\Delta t)}{1} + \vec{G}^*_{ji} \frac{(\Delta t)^2}{2}] \tag{4.33b}$$

The $\vec{G}^*_{ji}$ are to be chosen so that $\vec{G}^*_{ji} = -\vec{G}^*_{ij}$ and

$$\vec{G}^*_{ji} = \vec{G}_{ji} + O[\Delta t] \tag{4.34}$$

and so that $\vec{L}$ and E are maximally conserved. Using eqs. (4.33) and algebra similar to that of Sect. 4.A.i.,

$$\Delta\vec{L}_c = \frac{(\Delta t)^2}{2} \sum_{i<j} [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{G}_{ij} \times (\vec{v}_{ij} + \vec{a}_{ij} \Delta t) \frac{\Delta t}{3}$$

$$+ \vec{r}\,'_{c,ij} \times \vec{G}^*_{ij}] \tag{4.35}$$

where

$$\vec{r}\,'_{c,ij} = \vec{r}\,'_{c,j} - \vec{r}\,'_{c,i} \tag{4.36a}$$

$$= \vec{r}_{ij} + \vec{v}_{ij} \Delta t + \vec{a}_{ij} \frac{(\Delta t)^2}{2} + \vec{b}_{ij} \frac{(\Delta t)^3}{6} \tag{4.36b}$$

and

$$\vec{b}_{ij} = \sum_{k=1}^{n} \left(\frac{\vec{G}_{kj}}{m_j} - \frac{\vec{G}_{ki}}{m_i}\right) \tag{4.37}$$

As in Sect. 4.A.i. above, the $\vec{G}^*_{ij}$ are chosen to make each ij term in eq. (4.35) to vanish to as high an order as possible. Setting

$$\vec{r}\,'_{c,ij} \times [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{G}_{ij} \times (\vec{v}_{ij} + \vec{a}_{ij} \Delta t) \frac{\Delta t}{3}$$

$$+ \vec{r}\,'_{c,ij} \times \vec{G}^*_{ij}] = \vec{0} \tag{4.38}$$

and solving for the $\vec{G}^*_{ij}$ gives:

$$\vec{G}^{*}_{ij} = \epsilon_{ij}\, \vec{r}\,'_{c,ij} + \vec{\beta}_{ij} \tag{4.39}$$

where ϵ_{ij} is the (unknown) component of $\vec{G}^{*}_{ij}$ in the $\vec{r}\,'_{c,ij}$ direction, and

$$\vec{\beta}_{ij} = \frac{\vec{r}\,'_{c,ij} \times [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{G}_{ij} \times (\vec{v}_{ij} + \vec{a}_{ij}\, \Delta t)\, \frac{\Delta t}{3})]}{(r'_{c,ij})^2} \tag{4.40}$$

As in Sect. 4.A.i., it is interesting to examine the error in $\vec{L}$ which results from the choice (4.39) for the $\vec{G}^{*}_{ij}$. Since

$$\vec{r}\,'_{c,ij} \times \vec{G}^{*}_{ij} = \vec{r}\,'_{c,ij} \times \vec{\beta}_{ij} \tag{4.41a}$$

$$= \frac{\vec{r}\,'_{c,ij} \cdot [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{G}_{ij} \times (\vec{v}_{ij} + \vec{a}_{ij}\, \Delta t)\, \frac{\Delta t}{3}]}{(r'_{c,ij})^2}\, \vec{r}\,'_{c,ij}$$

$$- \vec{v}_{ij} \times \vec{F}_{ij} - \vec{G}_{ij} \times (\vec{v}_{ij} + \vec{a}_{ij}\, \Delta t)\, \frac{\Delta t}{3} \tag{4.41b}$$

then eq. (4.35) becomes (via eqs. (3.7b) and (4.36))

$$\Delta \bar{L}_c =$$

$$\frac{(\Delta t)^2}{2} \sum_{i<j} \vec{r}\,'_{c,ij} \cdot [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{G}_{ij} \times (\vec{v}_{ij} + \vec{a}_{ij}\, \Delta t)\, \frac{\Delta t}{3}]\, \frac{\vec{r}\,'_{c,ij}}{(r'_{c,ij})^2} \tag{4.42a}$$

$$= \frac{(\Delta t)^2}{2} \sum_{i<j} [\vec{a}_{ij} \cdot \vec{v}_{ij} \times \vec{F}_{ij} \frac{(\Delta t)^2}{2} + \vec{r}_{ij} \cdot \vec{G}_{ij} \times \vec{a}_{ij} \frac{(\Delta t)^2}{3}$$

$$+ O[(\Delta t)^3] \frac{\vec{r}\,'_{c,ij}}{(r'_{c,ij})^2} \tag{4.42b}$$

$$= \frac{(\Delta t)^4}{12} \sum_{i<j} [3\, \vec{a}_{ij} \cdot \vec{v}_{ij} \times \vec{F}_{ij} + 2\, \vec{r}_{ij} \cdot \vec{G}_{ij} \times \vec{a}_{ij}] \frac{\vec{r}\,'_{c,ij}}{(r'_{c,ij})^2} + O[(\Delta t)^5] \tag{4.42c}$$

$$= O[(\Delta t)^4] \tag{4.42d}$$

which is to be contrasted with the error of $O[(\Delta t)^3]$ of eq. (3.21) when $\vec{G}^*_{ij} = \vec{G}_{ij}$ in eqs. (3.12b). Of course, for the case of only a single interaction $(n = 2)$ each ij term in eq. (4.42) vanishes completely, leading to exact conservation of $\vec{L}$, agreeing with the results of Part I [8].

As in Sect. 4.A.i., the quantities ϵ_{ij} are determined from the criterion that ΔE_c vanish. The analogue to eq. (4.16) is

$$\Delta E_c =$$

$$\Delta t \sum_{i<j} [(\vec{v}_{ij} + \vec{a}_{ij}\, \Delta t + \vec{b}^*_{ij} \frac{(\Delta t)^2}{4}) \cdot \vec{G}^*_{ij} \frac{\Delta t}{2} + (\vec{v}_{ij} + \vec{a}_{ij} \frac{\Delta t}{2}) \cdot \vec{F}_{ij} + \frac{\Delta \phi_{ij}}{\Delta t}] \tag{4.43}$$

where

$$\vec{b}^*_{ij} = \sum_{k=1}^{n} \left(\frac{\vec{G}^*_{kj}}{m_j} - \frac{\vec{G}^*_{ki}}{m_i}\right) \tag{4.44}$$

The equations to be solved for the ϵ_{ij} are then

$$[(\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t+\vec{b}^{*}_{ij}\,\frac{(\Delta t)^2}{4}]\cdot\vec{G}^{*}_{ij}\,\frac{\Delta t}{2}+(\vec{v}_{ij}+\vec{a}_{ij}\,\frac{\Delta t}{2})\cdot\vec{F}_{ij}+\frac{\Delta\phi_{ij}}{\Delta t} = 0 \qquad (4.45)$$

for which the Newton iteration formula is

$$\epsilon^{(k+1)}_{ij} = \epsilon^{(k)}_{ij}-\frac{2}{\Delta t}\,\frac{(\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t+\vec{b}^{*}_{ij}\,\frac{(\Delta t)^2}{4})\cdot\vec{G}^{*}_{ij}\frac{\Delta t}{2}+(\vec{v}_{ij}+\vec{a}_{ij}\,\frac{\Delta t}{2})\cdot\vec{F}_{ij}+\frac{\Delta\phi_{ij}}{\Delta t}}{\vec{r}\,'_{c,ij}\cdot[\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t+\vec{b}^{*}_{ij}\,\frac{(\Delta t)^2}{4}+(\frac{1}{m_i}+\frac{1}{m_j})\vec{G}^{*}_{ij}\,\frac{(\Delta t)^2}{4}]}\Bigg|_k \qquad (4.46)$$

For small Δt eqs. (4.45) are again strongly linear with

$$\epsilon_{ij} = \epsilon^{(1)}_{ij} + O[(\Delta t)^2] \qquad (4.47)$$

and

$$\epsilon^{(1)}_{ij} = \frac{df_{ij}}{dr_{ij}}\,\dot{r}_{ij} + O[\Delta t] \qquad (4.48)$$

If eqs. (4.46) are iterated to convergence, exact conservation of energy will result, as compared to an error of $O[(\Delta t)^3]$ using the method of eqs. (3.12).

B. Implicit Formulation

Implicit maximally conservative methods can also be obtained by replacing, e.g., the $\vec{F}_{ij}$ in <u>both</u> the $\vec{r}'_{c,i}$ and $\vec{v}'_{c,i}$ by the $\vec{F}^*_{ij}$. This results in equations for the ϵ_{ij} which are <u>implicit</u> by virtue of the dependences of the form $\phi_{ij}(r'_{c,ij})$.

i. Second-Order Method

Consider the simple formulae of eqs. (3.10) with the $\vec{F}^*_{ij}$ replacing <u>both</u> occurrences of the $\vec{F}_{ij}$:

$$\vec{r}'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} \vec{F}^*_{ji} \frac{(\Delta t)^2}{2} \tag{4.49a}$$

$$\vec{v}'_{c,i} = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} \vec{F}^*_{ji} \Delta t \tag{4.49b}$$

The $\vec{F}^*_{ji}$ are to be chosen so that eq. (4.2) is satisfied and maximal conservation of E and $\vec{L}$ occurs. From eqs.(4.3a), replacing the $\vec{F}_{ij}$ with the $\vec{F}^*_{ij}$,

$$\Delta\vec{L}_c = \Delta t \sum_{i=1}^{n} \sum_{j=1}^{n} (\vec{r}_i + \vec{v}_i \frac{\Delta t}{2}) \times \vec{F}^*_{ji} \tag{4.50a}$$

$$= \Delta t \sum_{i<j} \vec{\alpha}_{ij} \times \vec{F}^*_{ij} \tag{4.50b}$$

where

$$\vec{\alpha}_{ij} = \vec{r}_{ij} + \vec{v}_{ij} \frac{\Delta t}{2} \tag{4.51}$$

Since each term in eq. (4.50b) is dependent upon a single $\bar{F}^*_{ij}$, exact conservation of $\bar{L}$ occurs if

$$\vec{F}^*_{ij} = \epsilon_{ij} \vec{\alpha}_{ij} \tag{4.52}$$

where ϵ_{ij} is arbitrary.

Similarly, the error ΔE_c in the energy is given by eqs. (4.16) with the $r'_{c,ij}$ implicitly dependent upon the $\vec{F}^*_{ij}$:

$$\Delta E_c = \Delta t \sum_{i<j} [(\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2}) \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}] \tag{4.53}$$

The equations to be solved for the ϵ_{ij} are then eqs. (4.19), with Newton-type iteration formulae given by

$$\epsilon^{(k+1)}_{ij} = \epsilon^{(k)}_{ij} - \left. \frac{(\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2}) \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}}{\vec{\alpha}_{ij} \cdot [\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2} + \frac{\Delta t}{2} (\frac{1}{m_i} + \frac{1}{m_j}) \vec{F}^*_{ij} - (\frac{1}{m_i} + \frac{1}{m_j}) \vec{F}^*_{ij} \frac{\Delta t}{2}]} \right|_k$$

(4.54a)

$$= \epsilon^{(k)}_{ij} - \left. \frac{(\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2}) \cdot \vec{F}^*_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}}{\vec{\alpha}_{ij} \cdot (\vec{v}_{ij} + \vec{a}^*_{ij} \frac{\Delta t}{2})} \right|_k \tag{4.54b}$$

$$= - \left. \frac{\Delta\phi_{ij}/\Delta t}{\vec{\alpha}_{ij} \cdot (\vec{v}_{ij} + \vec{a}^{*}_{ij} \frac{\Delta t}{2})} \right|_k \tag{4.54c}$$

$$= - \left. \frac{\Delta\phi_{ij}}{\vec{\alpha}_{ij} \cdot (\vec{r}\,'_{c,ij} - \vec{r}_{ij})} \right|_k \tag{4.54d}$$

Since

$$\vec{\alpha}_{ij} \cdot (\vec{r}\,'_{c,ij} - \vec{r}_{ij}) = \frac{\vec{r}\,'_{c,ij} + \vec{r}_{ij}}{2} \cdot (\vec{r}\,'_{c,ij} - \vec{r}_{ij}) + O[(\Delta t)^3] \tag{4.55a}$$

$$= r_{ij}(r'_{c,ij} - r_{ij}) + O[(\Delta t)^2] \tag{4.55b}$$

it is evident via eq. (4.54d) that eq. (4.26) and its subsequent discussion also holds for the ϵ_{ij} of this section.

These second-order formulae as developed in this section have the unique property of exactly conserving both the total energy and angular momentum for an arbitrary system of particles. Eqs. (4.49), along with eqs. (4.52) and (4.54), are equivalent to the "discrete mechanics" of [5].

ii. Third-Order Method

Replacing all occurrences of $\vec{G}_{ij}$ in eqs. (4.33) by $\vec{G}^{*}_{ij}$ gives the formulae

$$\vec{r}\,'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} [\vec{F}_{ji} \frac{(\Delta t)^2}{2} + \vec{G}^{*}_{ji} \frac{(\Delta t)^3}{6}] \tag{4.56a}$$

$$\vec{v}'_{c,i} = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} [\vec{F}_{ji} \Delta t + \vec{G}^*_{ji} \frac{(\Delta t)^2}{2}] \tag{4.56b}$$

The $\vec{G}^*_{ij}$ are to be chosen so that eq. (4.34) holds and E and $\vec{L}$ are maximally conserved.

The analogue of eq. (4.35) for the $\vec{G}^*_{ij}$ is

$$\Delta\vec{L}_c = \frac{(\Delta t)^2}{2} \sum_{i<j} [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{\alpha}_{ij} \times \vec{G}^*_{ij}] \tag{4.57}$$

where

$$\vec{\alpha}_{ij} = \vec{r}_{ij} + \vec{v}_{ij} \frac{2\Delta t}{3} + \vec{a}_{ij} \frac{(\Delta t)^2}{6} \tag{4.58}$$

Conservation of angular momentum in all directions except $\vec{\alpha}_{ij}$ occurs if

$$\vec{\alpha}_{ij} \times [\vec{v}_{ij} \times \vec{F}_{ij} + \vec{\alpha}_{ij} \times \vec{G}^*_{ij}] = \vec{0} \tag{4.59}$$

with solution

$$\vec{G}^*_{ij} = \epsilon_{ij} \vec{\alpha}_{ij} + \vec{\beta}_{ij} \tag{4.60}$$

where ϵ_{ij} is undetermined as yet and

$$\vec{\beta}_{ij} = \frac{\vec{\alpha}_{ij}}{\alpha^2_{ij}} \times (\vec{v}_{ij} \times \vec{F}_{ij}) \tag{4.61a}$$

$$= [(\vec{\alpha}_{ij} \cdot \vec{F}_{ij}) \vec{v}_{ij} - (\vec{\alpha}_{ij} \cdot \vec{v}_{ij}) \vec{F}_{ij}] / \alpha^2_{ij} \tag{4.61b}$$

With the choice of eq. (4.60) for the $\vec{G}^*_{ij}$, the resulting error $\Delta\vec{L}_c$ in the angular momentum is then, from eq. (4.57),

$$\Delta\vec{L}_c = \frac{(\Delta t)^2}{2} \sum_{i<j} \frac{\vec{\alpha}_{ij} \cdot (\vec{v}_{ij} \times \vec{F}_{ij})}{\alpha^2_{ij}} \vec{\alpha}_{ij} \tag{4.62a}$$

$$= \frac{(\Delta t)^4}{12} \sum_{i<j} \frac{\vec{a}_{ij} \cdot \vec{v}_{ij} \times \vec{F}_{ij}}{\alpha^2_{ij}} \vec{\alpha}_{ij} \tag{4.62b}$$

$$= O[(\Delta t)^4] \tag{4.62c}$$

Of course, for the case of a single interaction (n = 2), $\vec{a}_{ij}$ and $\vec{F}_{ij}$ are proportional and $\Delta\vec{L}_c$ vanishes completely, agreeing with the results of Part I [8].

The error ΔE_c in the calculated value of the energy is given by eqs. (4.43) with the $\phi'_{c,ij}$ implicitly depend upon the $\vec{G}^*_{ij}$:

$$\Delta E_c = \Delta t \sum_{i<j} [(\vec{v}_{ij} + \vec{a}_{ij}\,\Delta t + \vec{b}^*_{ij}\,\frac{(\Delta t)^2}{4})\cdot\vec{G}^*_{ij}\,\frac{\Delta t}{2} + (\vec{v}_{ij} + \vec{a}_{ij}\,\frac{\Delta t}{2})\cdot\vec{F}_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}] \tag{4.63}$$

with the $\vec{b}^*_{ij}$ given by eq. (4.44). The equations to be solved are

$$[\vec{v}_{ij} + \vec{a}_{ij}\,\Delta t + \vec{b}^*_{ij}\,\frac{(\Delta t)^2}{4}]\cdot\vec{G}^*_{ij}\,\frac{\Delta t}{2} + (\vec{v}_{ij} + \vec{a}_{ij}\,\frac{\Delta t}{2})\cdot\vec{F}_{ij} + \frac{\Delta\phi_{ij}}{\Delta t} = 0 \tag{4.64}$$

which are implicit in the ϵ_{ij}. The Newton-type iteration formulae for the ϵ_{ij} are

$$\epsilon_{ij}^{(k+1)} = \epsilon_{ij}^{(k)} - \frac{2}{\Delta t} \left. \frac{[\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t + \vec{b}_{ij}^{*}\,\frac{(\Delta t)^2}{4}]\cdot \vec{G}_{ij}^{*}\frac{\Delta t}{2} + (\vec{v}_{ij}+\vec{a}_{ij}\,\frac{\Delta t}{2})\cdot \vec{F}_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}}{\alpha_{ij}\cdot[\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t + \vec{b}_{ij}^{*}\,\frac{(\Delta t)^2}{4} + (\frac{1}{m_i}+\frac{1}{m_j})\vec{G}_{ij}^{*}\,\frac{(\Delta t)^2}{4} - (\frac{1}{m_i}+\frac{1}{m_j})(\vec{F}_{ij}+\vec{G}_{ij}^{*}\,\Delta t)\frac{\Delta t}{3}]} \right|_k \tag{4.65a}$$

$$= \epsilon_{ij}^{(k)} - \frac{2}{\Delta t} \left. \frac{[\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t + \vec{b}_{ij}^{*}\,\frac{(\Delta t)^2}{4}]\cdot \vec{G}_{ij}^{*}\frac{\Delta t}{2} + (\vec{v}_{ij}+\vec{a}_{ij}\,\frac{\Delta t}{2})\cdot \vec{F}_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}}{\vec{\alpha}_{ij}\cdot[\vec{v}_{ij}+\vec{a}_{ij}\,\Delta t + \vec{b}_{ij}^{*}\,\frac{(\Delta t)^2}{4} - (\frac{1}{m_i}+\frac{1}{m_j})(\vec{F}_{ij}+\vec{G}_{ij}^{*}\,\frac{\Delta t}{4})\frac{\Delta t}{3}]} \right|_k \tag{4.65b}$$

Eqs. (4.47) and (4.48) also hold for the ϵ_{ij} of this section.

5. Numerical Example

In this section a direct numerical comparison will be made, for the case of a particular three-body problem, between the third-order Adams' method of Sect. 3.B and the implicit, third-order, conservative method of Sect. 4.B.ii. Numerical results using the second-order method of Sect. 4.B.i. have been presented previously [5].

The case chosen was selected to mimic the reactive interaction of an atom with a diatomic molecule. Here n = 3 and

$$m_1 = m_2 = m_3 = 1 \tag{5.1}$$

The potentials of interaction ϕ_{12}, ϕ_{23}, and ϕ_{13} were all of the Lennard-Jones (12,6) form

$$\phi_{LJ}(r) = 4\left[\frac{1}{r^{12}} - \frac{1}{r^{6}}\right] \tag{5.2}$$

The initial conditions at t = 0 were

$$\vec{r}_1(0) = \langle -3., .5, 0 \rangle \tag{5.3a}$$

$$\vec{v}_1(0) = \langle 1., 0., 0. \rangle \tag{5.3b}$$

$$\vec{r}_2(0) = \langle -.7, -.7, -.7 \rangle \tag{5.3c}$$

$$\vec{v}_2(0) = \langle .1, -.1, 0. \rangle \tag{5.3d}$$

$$\vec{r}_3(0) = \langle .7, .7, .7 \rangle \tag{5.3e}$$

$$\vec{v}_3(0) = \langle .1, .1, .1 \rangle \tag{5.3f}$$

For these initial conditions, the total angular momentum is given by

$$\vec{L} = \langle -.07, \ -.07, \ -.36 \rangle \tag{5.4}$$

with magnitude

$$L = 0.3733630941 \tag{5.5}$$

The total energy is

$$E = 0.4934308709 \tag{5.6}$$

At $t = 0$, particles 2 and 3 are bound. As $t \to \infty$, particle 1 has reacted with particle 2, leaving particle 3 free. Two asymptotic ($t \to \infty$) quantities of interest are the internal energy E_{12} of the bound pair 12, defined by

$$E_{12} = \frac{1}{2} \frac{m_1 m_2}{m_1+m_2} (\vec{v}_{12} \cdot \vec{v}_{12}) + \phi_{12}(r_{12}) \tag{5.7}$$

and the relative translational energy $E_{3,12}$ of particle 3:

$$E_{3,12} = \frac{1}{2} \frac{m_3(m_1+m_2)}{m_1+m_2+m_3} \left| \vec{v}_3 - \frac{m_1\vec{v}_1+m_2\vec{v}_2}{m_1+m_2} \right|^2 \tag{5.8}$$

Both the method of Sect. 4.B.ii. and the Adams' method used a maximum step-size of $\Delta t = .01$. Smaller step-sizes were chosen only to insure adequate convergence of the implicit equations to a relative tolerance of 10^{-10} (In the method of Sect. 4.B.ii., this tolerance was on the value of ΔE_c.) Programs implementing the method of Sect. 4.B.ii. are given in the Appendix of [9]. The program for the Adams' method is given in the Appendix of [5b].

The calculated values obtained by the two methods for E_{12} and $E_{3,12}$ are given in Table I, for a value of t large enough that further three-body interactions were negligible. Also shown are the maximum observed errors $|\Delta E_c|$ and $|\Delta \vec{L}_c|$ in the energy and angular momentum, respectively.

TABLE I

Comparison of Conservative and Nonconservative Third-Order Methods

Quantity	Method of Sect. 4.B.ii	Adams' Method
t (final)	10.0	10.0
No. steps	1472	1000
E_{12} [a]	-0.004227	-0.004195
$E_{3,12}$ [b]	0.25602	0.25599
max. $\lvert \Delta E_c \rvert \times 10^{10}$	-34	-50592433
max. $\lvert \Delta \vec{L}_c \rvert \times 10^{10}$	+135	+5630880

---

[a] Correct value is $E_{12} = -0.004250$

[b] Correct value is $E_{3,12} = 0.25604$

6. Extension to Arbitrary Order

For completeness, we will now show how to extend the explicit and implicit methods of Sect. 4 to arbitrary order. The discussion is based upon the use of a truncated Taylor-series form, similar to that of Sect. 3.A. The development extends also to predictor-corrector methods in the Nordsieck form [10]. Similar results are easily obtained for other forms.

Let $\vec{F}_i^{(k)}$ denote the k-th time-derivative of the force $\vec{F}_i$:

$$\vec{F}_i^{(k)} = \frac{d^k\vec{F}_i}{dt^k} \tag{6.1}$$

The (m+2)-th order truncated Taylor-series approximations to $\vec{r}_i'$ and $\vec{v}_i'$ are

$$\vec{r}_i' = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{k=0}^{m} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} \tag{6.2a}$$

$$\vec{v}_i' = \vec{v}_i + \frac{1}{m_i} \sum_{k=0}^{m} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} \tag{6.2b}$$

The explicit formulation is given by eq. (6.2) with $\vec{F}_i^{(m)}$ in eq. (6.2b) replaced by an adjustable $\vec{F}_i^{(m)*}$:

$$\vec{r}_{c,i}' = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{k=0}^{m} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} \tag{6.3a}$$

$$\vec{v}'_{c,i} = \vec{v}_i + \frac{1}{m_i} \left[\sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} + \vec{F}_i^{(m)*} \frac{(\Delta t)^{m+1}}{(m+1)!} \right] \qquad (6.3b)$$

Noting that

$$m_i(\vec{r}'_{c,i} \times \vec{v}'_{c,i}) = m_i(\vec{r}_i \times \vec{v}_i) +$$

$$\sum_{k=0}^{m-1} [\vec{r}_i \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} + \vec{v}_i \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} (k+1)]$$

$$+ \frac{1}{m_i} \sum_{\ell>k}^{m-1} \vec{F}_i^{(\ell)} \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+\ell+3}}{(k+1)!\,(\ell+1)!} \left(\frac{1}{\ell+2} - \frac{1}{k+2}\right)$$

$$+ \vec{F}_i^{(m)} \times \left(\vec{v}_i + \frac{1}{m_i} \sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!}\right) \frac{(\Delta t)^{m+2}}{(m+2)!}$$

$$+ \vec{r}'_{c,i} \times \vec{F}_i^{(m)*} \frac{(\Delta t)^{m+1}}{(m+1)!} \qquad (6.4)$$

then

$$\Delta\vec{L}_c = \sum_{i=1}^{n} \left\{ \sum_{k=0}^{m-1} \left(\vec{r}_i + \vec{v}_i \frac{\Delta t(k+1)}{k+2}\right) \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} \right.$$

$$+ \frac{1}{m_i} \sum_{\ell>k}^{m-1} \vec{F}_i^{(\ell)} \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+\ell+3}(k-\ell)}{(k+2)!\,(\ell+2)!}$$

$$+ \vec{F}_i^{(m)} \times \left(\vec{v}_i + \frac{1}{m_i} \sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!}\right) \frac{(\Delta t)^{m+2}}{(m+2)!}$$

$$\left. + \vec{r}'_{c,i} \times \vec{F}_i^{(m)*} \frac{(\Delta t)^{m+1}}{(m+1)!} \right\} \qquad (6.5)$$

Since eqs. (6.3) are exact to order m+1 without the terms involving the $\vec{F}_i^{(m)}$, all terms in eq. (6.5) of $O[(\Delta t)^k]$ vanish for $k \leq m$. Thus eq. (6.5) reduces to

$$\Delta\vec{L}_c = \frac{(\Delta t)^{m+1}}{(m+1)!} \sum_{i=1}^{n} [m\,\vec{v}_i \times \vec{F}_i^{(m-1)}$$

$$+ \frac{1}{m_i} \sum_{k=0}^{m-1} \sum_{\substack{\ell > k \\ \ell = m-2-k}}^{m-1} \vec{F}_i^{(\ell)} \times \vec{F}_i^{(k)} \frac{(k-\ell)(m+1)!\,(\Delta t)^{k+\ell+2-m}}{(k+2)!\,(\ell+2)!}$$

$$+ \vec{F}_i^{(m)} \times (\vec{v}_i + \frac{1}{m_i} \sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!}) \frac{\Delta t}{m+2}$$

$$+ \vec{r}\,'_{c,i} \times \vec{F}_i^{(m)*}] \tag{6.6}$$

Now,

$$\vec{F}_i^{(k)} = \sum_{j=1}^{n} \vec{F}_{ji}^{(k)} \tag{6.7}$$

where

$$\vec{F}_{ji}^{(k)} = \frac{d^k \vec{F}_{ji}}{dt^k} \tag{6.8a}$$

$$= \begin{cases} -\vec{F}_{ij}^{(k)} & i \neq j \\ 0 & i = j \end{cases} \tag{6.8b}$$

Let

$$\vec{a}_{ij}^{(k)} = \frac{d^k \vec{a}_{ij}}{dt^k} \tag{6.9a}$$

$$= \sum_{\ell=1}^{n} \left(\frac{\vec{F}_{\ell j}^{(k)}}{m_j} - \frac{\vec{F}_{\ell i}^{(k)}}{m_i}\right) \tag{6.9b}$$

Transforming eq. (6.6) to the i<j form then gives

$$\Delta\vec{L}_c = \frac{(\Delta t)^{m+1}}{(m+1)!} \sum_{i<j} [m\,\vec{v}_{ij} \times \vec{F}_{ij}^{(m-1)}$$

$$+ \sum_{k=0}^{m-1} \sum_{\substack{\ell=m-2-k \\ \ell>k}}^{m-1} \vec{a}_{ij}^{(\ell)} \times \vec{F}_{ij}^{(k)} \frac{(k-\ell)(m+1)!\,(\Delta t)^{k+\ell+2-m}}{(k+2)!\,(\ell+2)!}$$

$$+ \vec{F}_{ij}^{(m)} \times (\vec{v}_{ij} + \sum_{k=0}^{m-1} \vec{a}_{ij}^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!}) \frac{\Delta t}{m+2}$$

$$+ \vec{r}\,'_{c,ij} \times \vec{F}_{ij}^{(m)*}] \tag{6.10}$$

Requiring each ij term to vanish when crossed with $\vec{r}\,'_{c,ij}$, and solving for $\vec{F}_{ij}^{(m)*}$, gives

$$\vec{F}_{ij}^{(m)*} = \epsilon_{ij}\, \vec{r}\,'_{c,ij} + \vec{\beta}_{ij} \tag{6.11}$$

where ϵ_{ij} is arbitrary and

$$\vec{\beta}_{ij} = \frac{\vec{r}'_{c,ij}}{(r'_{c,ij})^2} \times [m\,\vec{v}_{ij} \times \vec{F}_{ij}^{(m-1)}$$

$$+ \sum_{k=0}^{m-1} \sum_{\substack{\ell=m-2-k \\ \ell>k}}^{m-1} \vec{a}_{ij}^{(\ell)} \times \vec{F}_{ij}^{(k)} \frac{(k-\ell)(m+1)(\Delta t)^{\ell+k+2-m}}{(k+2)!\,(\ell+2)!}$$

$$+ \vec{F}_{ij}^{(m)} \times (\vec{v}_{ij} + \sum_{k=0}^{m-1} \vec{a}_{ij}^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!}) \frac{\Delta t}{m+2}] \tag{6.12}$$

The ϵ_{ij} are determined from the criterion $\Delta E_c = 0$, which necessitates

$$[\vec{v}_{ij} + \sum_{k=0}^{m-1} \vec{a}_{ij}^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} + \vec{a}_{ij}^{(m)*} \frac{(\Delta t)^{m+1}}{2(m+1)!}] \cdot \vec{F}_{ij}^{(m)*} \frac{(\Delta t)^{m}}{(m+1)!}$$

$$+ [\vec{v}_{ij} + \frac{1}{2} \sum_{k=0}^{m-1} \vec{a}_{ij}^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!}] \cdot \sum_{k=0}^{m-1} \vec{F}_{ij}^{(k)} \frac{(\Delta t)^{k}}{(k+1)!} + \frac{\Delta \phi_{ij}}{\Delta t} = 0 \tag{6.13}$$

These equations are strongly linear in the $\vec{F}_{ij}^{(m)*}$, and may be solved via Newton's method, as in Sect. 4.A.

It follows readily, for example, that setting m = 1 in the above formulas yields the method of Sect. 4.A.ii.

Next, for the implicit formulation, both occurrence of $\vec{F}_i^{(m)}$ in eqs. (6.2) are replaced by the adjustable $\vec{F}_i^{(m)*}$:

$$\vec{r}'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} + \vec{F}_i^{(m)*} \frac{(\Delta t)^{m+2}}{(m+2)!} \quad (6.14a)$$

$$\vec{v}'_{c,i} = \vec{v}_i + \frac{1}{m_i} \left[\sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} + \vec{F}_i^{(m)*} \frac{(\Delta t)^{m+1}}{(m+1)!} \right] \quad (6.14b)$$

From these formulae

$$m_i(\vec{r}'_{c,i} \times \vec{v}'_{c,i}) = m_i(\vec{r}_i \times \vec{v}_i) +$$

$$\sum_{k=0}^{m-1} \left[\vec{r}_i \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+1}}{(k+1)!} + \vec{v}_i \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2} (k+1)}{(k+2)!} \right]$$

$$+ \frac{1}{m_i} \sum_{\ell > k}^{m-1} \vec{F}_i^{(\ell)} \times \vec{F}_i^{(k)} \frac{(\Delta t)^{k+\ell+3} (k-\ell)}{(k+2)!\,(\ell+2)!}$$

$$+ \vec{\alpha}_i \times \vec{F}_{ij}^{(m)} \times \frac{(\Delta t)^{m+1}}{(m+1)!} \quad (6.15)$$

where

$$\vec{\alpha}_i = \vec{r}_i + \vec{v}_i \Delta t \frac{m+1}{m+2} +$$

$$+ \frac{1}{m_i} \sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} \left(1 - \frac{k+2}{m+2}\right) \quad (6.16a)$$

$$= \vec{r}_i + \vec{v}_i \frac{m+1}{m+2} \Delta t + \frac{1}{m_i} \sum_{k=0}^{m-1} \vec{F}_i^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} \frac{m-k}{m+2} \tag{6.16b}$$

Using formula (6.15), it follows, as for (6.10), that

$$\Delta \vec{L}_c = \frac{(\Delta t)^{m+1}}{(m+1)!} \sum_{i<j} [m \, \vec{v}_{ij} \times \vec{F}_{ij}^{(m-1)}$$

$$+ \sum_{k=0}^{m-1} \sum_{\substack{\ell=m-2-k \\ \ell>k}}^{m-1} \vec{a}_{ij}^{(\ell)} \times \vec{F}_{ij}^{(k)} \frac{(k-\ell)(m+1)!\,(\Delta t)^{k+\ell+2-m}}{(k+2)!\,(\ell+2)!}$$

$$+ \vec{\alpha}_{ij} \times \vec{F}_{ij}^{(m)*}] \tag{6.17}$$

where

$$\vec{\alpha}_{ij} = \vec{\alpha}_j - \vec{\alpha}_i \tag{6.18a}$$

$$= \vec{r}_{ij} + \vec{v}_{ij} \frac{m+1}{m+2} \Delta t + \sum_{k=0}^{m-1} \vec{a}_{ij}^{(k)} \frac{(\Delta t)^{k+2}}{(k+2)!} \frac{m-k}{m+2} \tag{6.18b}$$

Solving for the $\vec{F}_{ij}^{(m)*}$ yields

$$\vec{F}_{ij}^{(m)*} = \epsilon_{ij} \, \vec{\alpha}_{ij} + \vec{\beta}_{ij} \tag{6.19}$$

where

$$\vec{\beta}_{ij} = \frac{\vec{\alpha}_{ij}}{\alpha_{ij}^2} \times [m\,\vec{v}_{ij} \times \vec{F}_{ij}^{(m-1)}$$

$$+ \sum_{k=0}^{m-1} \sum_{\substack{\ell=m-2-k \\ \ell>k}}^{m-1} \vec{a}_{ij}^{(\ell)} \times \vec{F}_{ij}^{(k)} \frac{(k-\ell)(m+1)(\Delta t)^{k+\ell+2-m}}{(k+2)!\,(\ell+2)!} \qquad (6.20)$$

and the ϵ_{ij} are determined via the energy conservation conditions eqs. (6.13) where the $\phi'_{c,ij} = \phi_{ij}(r'_{c,ij})$ are implicitly dependent on the ϵ_{ij}.

It follows readily, for example, that setting $m = 1$ in the above formulas yields the method of Section 4.B.ii.

7. Remarks

Explicit and implicit methods for the numerical integration of equations of motion have been derived. These methods conserve the energy exactly, and the angular momentum to at least one higher order of approximation than conventional methods. The angular momentum is conserved exactly for the case of the second-order method of Sect. 4.B.ii., and by all the methods in the case of a single interaction.

This property of conservation of the constants of motion is expected to give these methods an exploitable advantage in the qualitative investigation of the motion of large systems of particles.

With regard to the extension of these methods to anisotropic and nonseparable potentials, see [6] and [7].

Finally, we note that the existence of higher-order conservative formulas which do conserve angular momentum exactly is still an open and important question.

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1. For a survey of pertinent topics, see:

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   (b) R. C. Tolman, The Principles of Statistical Mechanics, Oxford University Press, Oxford, 1938.

2. For reviews, see:

   (a) D. L. Bunker, "Classical Trajectory Methods", Methods of Computational Physics, vol. 10, p. 287, Academic Press, N.Y., 1971;

   (b) R. A. LaBudde, "Classical Mechanics of Molecular Collisions", University of Wisconsin Theoretical Chemistry Institute Report WIS-TCl-414 (1973).

3. See, e.g.:

   (a) A. E. Roy, Foundations of Astrodynamics, MacMillan, N.Y., 1965;

   (b) G. A. Chebotarev, Analytical and Numerical Methods of Celestial Mechanics, American Elsevier Publishing Co., N.Y., 1967.

4. See, e.g., the review by

   R. L. Duncombe, P. K. Seidelmann, and W. J. Klepczynski, "Dynamical Astronomy of the Solar System", Ann. Rev. of Astron. and Astrophys. <u>11</u>, 135 (1973).

5. R. A. LaBudde and D. Greenspan, "Discrete Mechanics - A General Treatment":

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6. R. A. LaBudde and D. Greenspan, "Discrete Mechanics for Anisotropic Potentials", University of Wisconsin, Computer Sciences Department Report WIS-CS-203 (1974).

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8. R. A. LaBudde and D. Greenspan, "Energy and Angular Momentum Conserving Methods of Arbitrary Order for the Numerical Integration of Equations of Motion. I. Motion of a Single Particle", University of Wisconsin Computer Sciences Department Report WIS-CS-208 (1974).

9. R. A. LaBudde and D. Greenspan, "Energy and Momentum Conserving Methods of Arbitrary Order for the Numerical Integration of Equations of Motion. II. Motion of a System of Particles", University of Wisconsin Computer Sciences Department Report WIS-CS-215 (1974).

10. See, e.g.,

    (a) A. Nordsieck, "Numerical Solution of Ordinary Differential Equations", Math. Comp., 16, 22 (1962);

    (b) C. W. Gear, Numerical Initial Value Problems in Ordinary Differential Equations, Sect. 9.2.5, Prentice-Hall, Englewood Cliffs, N.J., 1971;

    (c) R. A. LaBudde, "Extension of Nordsieck's Methods to the Numerical Solution of Higher-Order Ordinary Differential Equations", University of Wisconsin Theoretical Chemistry Institute Report WIS-TCI-443 (1971)

```
LATUD,9724,3CCC0F5203,5,10C
C TEST
N-MACC 1.14S-07/08/74-19:38:37 (,C)        TEST
            IMPLICIT REAL*8(A-H,O-Z)
            REAL*8 LX,LY,LZ,LMAC
            DIMENSION R(3,10,5),RIJ(3,45,4),AUX(3,45,4),POT(45,3),XMASS(10)
            DATA (POT(K,5),K=1,45)/45*2.D0/
            DATA ((R(I,J,1),I=1,3),J=1,3)/-3.D0,0.5D0,0.D0,3*-0.7D0,3*0.7D0/
            DATA ((R(I,J,2),I=1,3),J=1,3) /1.D0,2*0.D0,0.1D0,-0.1D0,0.D0,0.1D0
           1,0.1D0,0.1D0/
            DATA XMASS/10*1.D0/
            DATA NPART/3/,NDIM/3/
            DATA ETOL/1.D-10/,MAXIT/5/
            DATA ERRTOL/1.D+3/,HMIN/1.D-6/,HMAX/0.01D0/
            ISTEP = 0
            T = 0.D0
            H = 0.01D0
            NTOT = (NPART*(NPART-1))/2
            CALL TIMSET (0.)
            PRINT 5
      5     FORMAT (1H1)
      200   IF (ISTEP .NE. 20*(ISTEP/20) ) GO TO 700
            CALL TIMGET ('NEXT')
            PRINT 40,T,H,IER,ISTEP
      40    FORMAT (  5X,'TIME =',D15.5,D15.5,I5,5X,'STEP =',I5)
            CALL RVECT (R,R(1,1,2),RIJ,RIJ(1,1,2),POT(1,2),NDIM,NPART,3)
      10    FORMAT (5X,12F10.6)
            CALL POTVAL (POT(1,2),AUX,POT,NTOT,0)
            E = 0.D0
            DO 400 I = 1,NPART
            SUM = 0.D0
            DO 300 L = 1,NDIM
      300   SUM = SUM + R(L,I,2)*R(L,I,2)
      400   E = E + XMASS(I)*SUM
            E = 0.5D0*E
            DO 500 I = 1,NTOT
      500   E = E + POT(I,1)
            PRINT 20,E,(POT(I,2),I=1,NTOT)
      20    FORMAT ( 5X,'ENERGY =',D20.10,5X,3D21.10)
            LX = 0.D0
            LY = 0.D0
            LZ = 0.D0
            DO 600 I = 1,NPART
            LX = LX + XMASS(I)*(R(2,I,1)*R(3,I,2)-R(3,I,1)*R(2,I,2))
            LY = LY + XMASS(I)*(R(3,I,1)*R(1,I,2)-R(1,I,1)*R(3,I,2))
      600   LZ = LZ + XMASS(I)*(R(1,I,1)*R(2,I,2)-R(2,I,1)*R(1,I,2))
            LMAC = DSQRT(LX*LX + LY*LY + LZ*LZ)
            PRINT 30,LX,LY,LZ,LMAC
      30    FORMAT ( 5X,'ANG. MOMENTUM VECTOR',3D20.12,5X,'MAG.',D20.12)
      700   CALL DMASTR  (H,T,R,RIJ,AUX,POT,XMASS,ETOL,MAXIT,ERRTOL,NDIM,
           1 NPART,3,10,45,HMIN,HMAX,IER)
```

```
            ISTEP = ISTEP + 1
      900   IF (T .LT. 10.D0) GO TO 200
            CALL TIMEST ('END')
            PRINT 40,T,H,IER,ISTEP
            PRINT 50,(((R(L,I,J),J=1,5),L=1,3),I=1,3)
       50   FORMAT (5X,5D20.10)
            STOP
            END

END OF COMPILATION:          NO  DIAGNOSTICS.

 POTVAL
I-MACC 1.145-07/03/74-13:39:49 (,D)          POTVAL
            SUBROUTINE POTVAL (R,F,POT,NIJ,ISW)
            IMPLICIT REAL*8 (A-H,O-Z)
            DIMENSION R(1),F(1),POT(1)
            DO 100 I = 1,NIJ
            DODA = 1.D0/R(I)**6
            POT(I) = 4.D0*DODA*(DODA - 1.D0)
      100   IF (ISW .NE. 0) F(I) = 24.D0*DODA*(1.D0-2.D0*DODA)/R(I)
            RETURN
            END

END OF COMPILATION:          NO  DIAGNOSTICS.

 DMASTR
I-MACC 1.145-07/03/74-13:39:53 (,D)          DMASTR
            SUBROUTINE DMASTR  (H,T,R,RIJ,AUX,POT,XMASS,ETOL,MAXIT,ERRTOL,NDIM
           1,NPART,NSUB1,NSUB2,NSUB3,HMIN,HMAX,IDOUBL)
      C     CONTROLS STEPSIZE OF DM3 ROUTINE INTEGRATION
      C     ERRTOL - BOUND ON ERROR IN VELOCITY OF ANY PARTICLE
      C     HMIN - MINIMUM ALLOWABLE ABSOLUTE VALUE OF STEPSIZE H
      C     HMAX - MAXIMUM ALLOWABLE ABS. VALUE OF STEP H
      C     IDOUBL - IF 1, STEP H CAN BE DOUBLED NEXT TIME
            IMPLICIT REAL*8 (A-H,O-Z)
            DIMENSION R(NSUB1,NSUB2,4)
            IF (IDOUBL .LT. 1 .OR. DABS(2.D0*H) .GE. 1.0000001D0*HMAX) GO TO
           1 90
            H = 2.D0*H
            IDOUBL = -1
            GO TO 100
       90   IDOUBL = 0
      100   CALL DM3 (H,T,R,RIJ,AUX,POT,XMASS,ETOL,MAXIT,NDIM,NPART,NSUB1,
           1 NSUB2,NSUB3,IER)
            IF (IER .NE. 0) GO TO 400
            ERR = 0.D0
            DO 300 I = 1,NPART
            DO 300 J = 1,NDIM
      300   IF (ERR .LT. DABS(R(J,I,4)) ) ERR = DABS(R(J,I,4) )
            ERR = H*H*ERR
            IF (ERR .GT. ERRTOL) GO TO 400
            IF (4.D0*ERR .LT. ERRTOL) IDOUBL = IDOUBL + 1
            RETURN
      400   H = 0.5D0*H
            IDOUBL = IDOUBL - 1
            IF (DABS(H) .GE. HMIN) GO TO 100
            PRINT 10,H,HMIN,T
       10    FORMAT (///5X,'H =',D15.6,5X,'HMIN =',D15.6,5X,'T =',D15.6)
            STOP
```

```
                END

END OF COMPILATION:        NO  DIAGNOSTICS.
I DM3
J-MACC 1.14S-07/09/74-19:38:59 (,0)            DM3
                SUBROUTINE DM3(H,T,R,RIJ,AUX,POT,XMASS,ETOL,MAXIT,NDIM,NPART,NSUB1
               1,NSUB2,NSUB3,IER)
      C         H IS FIXED STEP-SIZE AND T IS CURRENT TIME
      C         NPART IS NO. OF PARTICLES IN SYSTEM AND NDIM IS NO. OF DIMENSIONS
      C         NOTE -- NSUB1 SHOULD BE GE NDIM, NSUB2 GE NPART AND NSUB3 GE
      C            NPART*(NPART-1)/2
                IMPLICIT REAL*8 (A-H,O-Z)
                DIMENSION R(NSUB1,NSUB2,5),RIJ(NSUB1,NSUB3,4),AUX(NSUB1,NSUB3,4),
               1 POT(NSUB3,5),XMASS(1)
                NIJ = (NPART*(NPART-1))/2
                H2 = 0.5DO*H
                H3 = 0.33333333333333333300*H
                H23 = C.66666666666666666700*H
                H4 = 0.25DO*H
                CALL RVECT (R,R(1,1,2),RIJ,RIJ(1,1,2),POT(1,3),NDIM,NPART,NSUB1)
      C         CALCULATE FORCES AND POTENTIALS AT OLD TIME
                CALL FORCE (RIJ(1,1,1),AUX,POT(1,3),POT(1,1),NDIM,NIJ,NSUB1,1)
                CALL ACCEL(R(1,1,3),AUX,XMASS,NDIM,NPART,NSUB1)
                CALL ACALC (R(1,1,3),RIJ(1,1,3),NDIM,NPART,NSUB1)
                ITER = 0
                IER = 0
                DO 400 K = 1,NIJ
                ALPMAG = 0.D0
                AF = 0.D0
                AV = 0.D0
      C         CALCULATE ALPHA(I,J) AND STORE IN AUX(L,K,3)
                DO 200 L = 1,NDIM
                DODA = RIJ(L,K,1) + H23*(RIJ(L,K,2) + H4*RIJ(L,K,3))
                AUX(L,K,3) = DODA
                ALPMAG = ALPMAG + DODA*DODA
                AF = AF + DODA*AUX(L,K,1)
      200       AV = AV + DODA*RIJ(L,K,2)
                POT(K,4) = 0.D0
      C         CALCULATE BETA(I,J) AND STORE IN AUX(L,K,4)
                DO 400 L = 1,NDIM
                DODA = (AF*RIJ(L,K,2)-AV*AUX(L,K,1))/ALPMAG
                AUX(L,K,4) = DODA
      400       POT(K,4) = POT(K,4) + AUX(L,K,1)*(RIJ(L,K,2)+H2*RIJ(L,K,3))
      C         FIRST ESTIMATE FOR EPSIJ IS PREVIOUS STEP'S VALUE
                DO 450 K = 1,NIJ
                DO 450 L = 1,NDIM
      450       AUX(L,K,2) = POT(K,5)*AUX(L,K,3) + AUX(L,K,4)
                CALL ACCEL (R(1,1,4),AUX(1,1,2),XMASS,NDIM,NPART,NSUB1)
      500       CALL ACALC (R(1,1,4),RIJ(1,1,4),NDIM,NPART,NSUB1)
                DO 800 K = 1,NIJ
                POT(K,3) = 0.D0
      C         CALCULATE R(I,J) AT NEW TIME AND STORE IN RIJ(L,K,5)
                DO 700 L = 1,NDIM
                DODA = RIJ(L,K,1) + H*(RIJ(L,K,2) + H2*(RIJ(L,K,3) + H3*RIJ(L,K,4
               1))
                RIJ(L,K,5) = DODA
      700       POT(K,3) = POT(K,3) + DODA*DODA
```

```
900   POT(K,3) = DSQRT(POT(K,3))
C     CALCULATE POTENTIAL AT NEW TIME
      CALL FORCE (RIJ(1,1,5),AUX,POT(1,3),POT(1,2),NDIM,NIJ,NSUB1,0)
      DELE = 0.D0
      DO 1100 K = 1,NIJ
C     CALCULATE EPS(I,J)
      DENOM = 0.D0
      TOP = 0.D0
      DO 1000 L = 1,NDIM
      TEMP = RIJ(L,K,2) + H*(RIJ(L,K,3) + H4*RIJ(L,K,4))
      TOP = TOP + TEMP*AUX(L,K,2)
1000  DENOM = DENOM + AUX(L,K,3)*(TEMP - POT(K,6)*(AUX(L,K,1)+H4*
     1 AUX(L,K,2))*H3 )
      TOP = H2*TOP + POT(K,4) + (POT(K,2)-POT(K,1))/H
      DELE = DELE + TOP
      POT(K,5) = POT(K,5) - TOP/(H2*DENOM)
C     CALCULATE D F(I,J)/DT
      DO 1100 L = 1,NDIM
1100  AUX(L,K,2) = POT(K,5)*AUX(L,K,3) + AUX(L,K,4)
      CALL ACCEL (R(1,1,4),AUX(1,1,2),XMASS,NDIM,NPART,NSUB1)
      IF (DABS(DELE*H) .LT. ETOL) GO TO 1400
      ITER = ITER + 1
      IF (ITER .LT. MAXIT) GO TO 500
      IER = 1
      RETURN
C     UPDATE TIME, POSITIONS, AND VELOCITIES
1400  T = T + H
      DO 1500 I = 1,NPART
      DO 1500 L = 1,NDIM
      R(L,I,1) = R(L,I,1) + H*(R(L,I,2) + H2*(R(L,I,3) + H3*R(L,I,4)))
1500  R(L,I,2) = R(L,I,2) + H*(R(L,I,3) + H2*R(L,I,4))
      RETURN
      END
```

END OF COMPILATION: NO DIAGNOSTICS.

FORCE

V-MACC 1.14S-07/09/74-19:39:06 (,0)   FORCE

```
      SUBROUTINE FORCE (RIJ,FIJ,RMAG,POT,NDIM,NIJ,NSUB,ISW)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION RIJ(NSUB,1),FIJ(1),RMAG(1),POT(1)
      CALL POTVAL (RMAG,FIJ,POT,NIJ,ISW)
      IF (ISW .EQ. 0) RETURN
C     IF ISW .NE. 0, CALCULATE FORCES
      K = NIJ + 1
100   K = K - 1
      IF (K .LE. 0) RETURN
      IJ = NSUB*(K-1)
      DODA = FIJ(K)/RMAG(K)
      L = NDIM
200   FIJ(IJ+L) = -DODA*RIJ(L,K)
      L = L - 1
      IF (L .GT. 0) GO TO 200
      GO TO 100
      END
```

END OF COMPILATION: NO DIAGNOSTICS.

RVECT

```
IN-MACC 1.14S-07/09/74-19:39:08 (,0)        RVECT
        SUBROUTINE RVECT (R,V,RIJ,VIJ,RMAG,NDIM,NPART,NSUB)
        IMPLICIT REAL*8 (A-H,O-Z)
        DIMENSION R(NSUB,1),V(NSUB,1),RIJ(NSUB,1),VIJ(NSUB,1),RMAG(1)
        K = 0
        DO 300 J = 2,NPART
        I = 0
  100   I = I + 1
        IF (I .GE. J) GO TO 300
        K = K + 1
        SUM = 0.D0
        DO 200 L = 1,NDIM
        RIJ (L,K) = R(L,J) - R(L,I)
        SUM = SUM + RIJ(L,K)*RIJ(L,K)
  200   VIJ(L,K) = V(L,J) - V(L,I)
        RMAG(K) = DSQRT(SUM)
        GO TO 100
  300   CONTINUE
        RETURN
        END

END OF COMPILATION:          NO DIAGNOSTICS.
SI ACCEL
IN-MACC 1.14S-07/09/74-19:39:13 (,0)        ACCEL
        SUBROUTINE ACCEL (A,FIJ,XMASS,NDIM,NPART,NSUB)
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION A(NSUB,1),FIJ(NSUB,1),XMASS(1)
        DO 400 I = 1,NPART
        NI = ((I-1)*(I-2))/2
        DO 400 L = 1,NDIM
        A(L,I) = 0.D0
        J = I
  100   J = J + 1
        IF (J .GT. NPART) GO TO 200
        K = ((J-1)*(J-2))/2 + I
        A(L,I) = A(L,I) - FIJ(L,K)
        GO TO 100
  200   J = 0
  300   J = J + 1
        IF (J .GE. I) GO TO 400
        K = NI + J
        A(L,I) = A(L,I) + FIJ(L,K)
        GO TO 300
  400   A(L,I) = A(L,I)/XMASS(I)
        RETURN
        ENTRY ACALC (A,FIJ,NDIM,NPART,NSUB)
        DO 700 I = 2,NPART
        NI = ((I-1)*(I-2))/2
        J = 0
  500   J = J + 1
        IF (J .GE. I) GO TO 700
        K = NI + J
        DO 600 L = 1,NDIM
  600   FIJ(L,K) = A(L,I) - A(L,J)
        GO TO 500
  700   CONTINUE
        RETURN
        END
```