DIRECT INTEGRATION METHODS OF THE *N*-BODY PROBLEM

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Abstract. A fourth-order polynomial method for the integration of *N*-body systems is described in detail together with the computational algorithm. Most particles are treated efficiently by an individual time-step scheme but the calculation of close encounters and persistent binary orbits is rather time-consuming and is best performed by special techniques. A discussion is given of the Kustaanheimo-Stiefel regularization procedure which is used to integrate dominant two-body encounters as well as close binaries. Suitable decision-making parameters are introduced and a simple method is developed for regularizing an arbitrary number of simultaneous two-body encounters.

1. Introduction

Numerical integrations of the gravitational *N*-body problem may in principle be performed by the simple method of advancing all equations of motion stepwise in time using constant forces. Any desired accuracy may be obtained by an appropriate choice of the time interval as long as rounding errors remain small. In view of the lengthy force calculation for large particle numbers it is desirable to employ high-order schemes which allow the choice of greater intervals. More powerful methods have also been developed for dealing with special configurations which would otherwise lead to serious loss of accuracy, or at best require very time-consuming calculations.

The present paper describes in some detail an ordinary fourth-order polynomial method as well as the Kustaanheimo-Stiefel regularization procedure for studying close two-body encounters. Although the former is very efficient in general circumstances, it is desirable to include special treatments of critical cases. Alternative regularization formulations are discussed elsewhere in this volume (Szebehely and Bettis, 1972; Heggie, 1972). A classical perturbation treatment of close binaries is also available, but this method is more suitable for small perturbations (Aarseth, 1970). Several types of ordinary integration schemes have been used for direct *N*-body calculations but high order polynomial methods appear to be the most efficient tried so far (Lecar, 1968).

2. Individual Time-Step Method

The motivation for introducing an individual time-step method stems from the desire to solve the equations of motion to the same relative accuracy in the absence of rounding errors. The resulting saving of force summations speeds up the calculations by a large factor, while the additional requirement of co-ordinate prediction only represents 20–30% of the total computing time depending on the order used.

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In the present formulation which follows an earlier derivation (Aarseth, 1968) we make explicit use of the first four terms of a fitting polynomial, but an additional correction term is included. Practical tests indicate that there is no significant gain in efficiency when going to higher orders, but an equivalent general derivation is available (Wielen, 1967).

We begin by writing the extrapolating force polynomial for an arbitrary body as an expansion about the reference time t_0, with the interval $t_r = t - t_0$,

$$\mathbf{F} = \mathbf{F}_0 + \mathbf{B}' t_r + \mathbf{C}' t_r^2 + \mathbf{D}' t_r^3 + \mathbf{E}' t_r^4 . \tag{1}$$

The coefficients $\mathbf{B}'$, $\mathbf{C}'$, $\mathbf{D}'$ are obtained by fitting the polynomial at three previous times and can be expressed in terms of higher divided differences at the time $t = t_0$ weighted by the corresponding intervals, while $\mathbf{F}_0$ represents the force per unit mass. Let the three preceding time-steps be denoted by Δt_1, Δt_2, Δt_3 in sequential order such that Δt_3 is the most recent interval. The force expansion (1) is then considered valid over the time interval $-(\Delta t_1 + \Delta t_2 + \Delta t_3) \leqslant t_r \leqslant \Delta t_4$, but the coefficient $\mathbf{E}'$ is not known until the end of the fourth step Δt_4 when its contribution is added. This procedure may be referred to as a semi-iteration since the main part of the improvement is achieved without recalculating the force which is based on the predicted position. In this way almost one extra order of integration is included at very little additional effort and only one force calculation is needed for each interval.

It is more convenient for computational purposes to write Equation (1) in the form

$$\begin{aligned} \mathbf{F} = \mathbf{F}_0 &+ \mathbf{B} t_r + \mathbf{C}(\Delta t_3 + t_r)\, t_r + \mathbf{D}(\Delta t_2 + \Delta t_3 + t_r)(\Delta t_3 + t_r)\, t_r \\ &+ \mathbf{E}(\Delta t_1 + \Delta t_2 + \Delta t_3 + t_r)(\Delta t_2 + \Delta t_3 + t_r)(\Delta t_3 + t_r)\, t_r . \end{aligned} \tag{2}$$

Explicit expressions for the coefficients $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ may then be obtained in terms of the divided backwards differences $\hat{\mathbf{F}}_0$, $\hat{\hat{\mathbf{F}}}_0$, $\hat{\hat{\hat{\mathbf{F}}}}_0$ defined by

$$\hat{\mathbf{F}}_0 = \frac{\mathbf{F}_0 - \mathbf{F}_{-3}}{\Delta t_3}, \quad \hat{\hat{\mathbf{F}}}_0 = \frac{\hat{\mathbf{F}}_0 - \hat{\mathbf{F}}_{-3}}{\Delta t_3}, \quad \hat{\hat{\hat{\mathbf{F}}}}_0 = \frac{\hat{\hat{\mathbf{F}}}_0 - \hat{\hat{\mathbf{F}}}_{-3}}{\Delta t_3} \tag{3}$$

where the force at time $t_r = -\Delta t_3$ is denoted by $\mathbf{F}_{-3}$. The adopted expressions take the final form

$$\mathbf{B} = \hat{\mathbf{F}}_0, \quad \mathbf{C} = \frac{\Delta t_3}{\Delta t_2 + \Delta t_3}\, \hat{\hat{\mathbf{F}}}_0 \tag{4}$$

$$\begin{aligned} \mathbf{D} = &\frac{\Delta t_2 \Delta t_3}{(\Delta t_1 + \Delta t_2 + \Delta t_3)(\Delta t_1 + \Delta t_2)}\, \hat{\hat{\hat{\mathbf{F}}}}_0 \\ &- \frac{\Delta t_2^2 - \Delta t_1 \Delta t_3}{(\Delta t_1 + \Delta t_2 + \Delta t_3)(\Delta t_1 + \Delta t_2)(\Delta t_2 + \Delta t_3)}\, \hat{\hat{\mathbf{F}}}_0 \end{aligned}$$

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$$\mathbf{E} = \frac{\dfrac{\Delta t_4}{\Delta t_3 + \Delta t_4}\overset{\wedge\wedge}{\mathbf{F}}_4 - \dfrac{\Delta t_3}{\Delta t_2 + \Delta t_3}\overset{\wedge\wedge}{\mathbf{F}}_0}{(\Delta t_1 + \Delta t_2 + \Delta t_3 + \Delta t_4)(\Delta t_2 + \Delta t_3 + \Delta t_4)} - \frac{\mathbf{D}}{(\Delta t_1 + \Delta t_2 + \Delta t_3 + \Delta t_4)},$$

where the coefficient $\mathbf{E}$ contains the divided difference $\overset{\wedge\wedge}{\mathbf{F}}_4$ equivalent to $\overset{\wedge\wedge}{\mathbf{F}}_0$ evaluated at $t_r = \Delta t_4$.

3. Computational Algorithm

The integrations may be started by first calculating the Taylor series derivatives from explicit differentiation of the equation of motion for each particle i,

$$\ddot{\mathbf{r}}_i = -\sum_{\substack{j=1 \\ j\neq i}}^{N} m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}, \tag{5}$$

where $\mathbf{F}_0 = \ddot{\mathbf{r}}_i$ by the notation above. Denoting Taylor series derivatives by dots and writing $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$, we obtain the relations (Gonzalez and Lecar, 1968)

$$\begin{aligned}
\dot{\mathbf{F}}_0 &= -\sum_j m_j \left\{ \frac{\dot{\mathbf{r}}_{ij}}{r_{ij}^3} - \frac{3\mathbf{r}_{ij}(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})}{r_{ij}^5} \right\} \\
\ddot{\mathbf{F}}_0 &= -\sum_j m_j \left\{ \frac{\ddot{\mathbf{r}}_{ij}}{r_{ij}^3} - \frac{6\dot{\mathbf{r}}_{ij}(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})}{r_{ij}^5} + \frac{3\mathbf{r}_{ij}}{r_{ij}^5}\left[\frac{5(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})^2}{r_{ij}^2} - \dot{\mathbf{r}}_{ij}\cdot\dot{\mathbf{r}}_{ij} - \mathbf{r}_{ij}\cdot\ddot{\mathbf{r}}_{ij} \right] \right\} \\
\dddot{\mathbf{F}}_0 &= -\sum_j m_j \left\{ \frac{\dddot{\mathbf{r}}_{ij}}{r_{ij}^3} - \frac{9\ddot{\mathbf{r}}_{ij}(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})}{r_{ij}^5} - \frac{\dot{\mathbf{r}}_{ij}}{r_{ij}^5}\left[9\dot{\mathbf{r}}_{ij}\cdot\dot{\mathbf{r}}_{ij} + 9\mathbf{r}_{ij}\cdot\ddot{\mathbf{r}}_{ij} - \frac{45(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})^2}{r_{ij}^2} \right] - \right. \\
&\quad - \frac{\mathbf{r}_{ij}}{r_{ij}^5}\left[3\mathbf{r}_{ij}\cdot\dddot{\mathbf{r}}_{ij} + 9\dot{\mathbf{r}}_{ij}\cdot\ddot{\mathbf{r}}_{ij} - \frac{45(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})(\mathbf{r}_{ij}\cdot\ddot{\mathbf{r}}_{ij})}{r_{ij}^2} - \right. \\
&\quad \left. \left. - \frac{45(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})(\dot{\mathbf{r}}_{ij}\cdot\dot{\mathbf{r}}_{ij})}{r_{ij}^2} + \frac{105(\mathbf{r}_{ij}\cdot\dot{\mathbf{r}}_{ij})^3}{r_{ij}^4} \right] \right\}.
\end{aligned} \tag{6}$$

Thus the second and third derivatives are readily determined once all the current forces and the corresponding first derivatives have been calculated.

Initial time-steps must now be allocated to each particle and a simpler form of the general criterion is used for this purpose. Usually it is sufficient to adopt

$$\Delta t_4^3 = \eta \frac{F_0}{\frac{1}{6}\dot{F}_0} \tag{7}$$

with $F_0 = |\mathbf{F}_0|$, etc. The parameter η specifies the permissible relative change of force during the new step as contributed by the last known term and hence controls the convergence of the Taylor series expansion. The definition (7) is independent of mass and has the desired property of preserving the relative accuracy of each orbit during close encounters by reducing the integration interval. Although the integration proper

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starts at the time $t=0$, it is necessary to initialize the previous steps in order to make use of the general formulation; hence we put

$$\Delta t_k = \Delta t_4 \quad (k=1,2,3), \tag{8}$$

where again the index i has been suppressed. A consistent conversion to polynomial derivatives is then readily obtained from the general relations

$$\begin{aligned}
\hat{\mathbf{F}}_0 &= \dot{\mathbf{F}}_0 - \tfrac{1}{2}\ddot{\mathbf{F}}_0\Delta t_3 + \tfrac{1}{6}\dddot{\mathbf{F}}_0\Delta t_3^2, \\
\hat{\hat{\mathbf{F}}}_0 &= \tfrac{1}{2}\ddot{\mathbf{F}}_0(\Delta t_2 + \Delta t_3)/\Delta t_3 - \tfrac{1}{6}\dddot{\mathbf{F}}_0(\Delta t_2 + 2\Delta t_3)(\Delta t_2 + \Delta t_3)/\Delta t_3, \\
\hat{\hat{\hat{\mathbf{F}}}}_0 &= \hat{\hat{\mathbf{F}}}_0 \frac{\Delta t_2^2 - \Delta t_1 \Delta t_3}{(\Delta t_2 + \Delta t_3)\Delta t_2 \Delta t_3} + \tfrac{1}{6}\dddot{\mathbf{F}}_0 \frac{(\Delta t_1 + \Delta t_2 + \Delta t_3)(\Delta t_1 + \Delta t_2)}{\Delta t_2 \Delta t_3}.
\end{aligned} \tag{9}$$

In order to proceed with the individual time-step scheme each particle must be assigned the time t_i of the most recent force computation. The remaining part of the interval is introduced as an auxiliary quantity

$$\Delta \tilde{t}_i = t_i + \Delta t_i - t \tag{10}$$

where the current step is denoted by Δt_i rather than the previous definition Δt_4.

The integration is continued by finding the index α with the smallest value of $\Delta \tilde{t}_i$,

$$\Delta \tilde{t}_\alpha = \min_i(\Delta \tilde{t}_i), \tag{11}$$

which determines the next particle to be considered. Advancing the time t to $t+\Delta \tilde{t}_\alpha$, all quantities $\Delta \tilde{t}_i$ are subtracted by $\Delta \tilde{t}_\alpha$ in order to be consistent with the definition (10). The body $i=\alpha$ now requires a new force determination but first all co-ordinates are predicted by low-order extrapolation. Increments to the positions are written as

$$\Delta \mathbf{r}_i = [(\tfrac{1}{6}\hat{\mathbf{F}}_0\Delta t_i' + \tfrac{1}{2}\mathbf{F}_0)\Delta t_i' + \dot{\mathbf{r}}_0]\Delta t_i', \tag{12}$$

where $\Delta t_i' = t - t_i$ is the time interval since the previous force computation. If Δt_α is small, the calculation of dominant force terms may be improved by including one extra order in the co-ordinate prediction for any other particles with small steps.

A more accurate position for the body $i=\alpha$ is obtained by integrating twice the increments from the coefficients C and D defined by Equation (4), after which the new force is calculated by the summation (5). The whole contribution from the fifth term of Equation (2) is now added as an improvement and the new velocity is obtained in a consistent manner by integrating the force polynomial once. At this stage it is convenient to initialize the individual reference time; i.e., $t_\alpha = t$, and update the quantities Δt_1, Δt_2, Δt_3 for the particle considered. Finally, the next time-step is predicted from the relative criterion

$$\Delta t_\alpha^3 = \eta\left[\frac{F_0 + \dot{F}_0\Delta t_3}{\tfrac{1}{6}\dddot{F}_0 + \tfrac{1}{24}F_0^{(\mathrm{IV})}\Delta t_3}\right], \tag{13}$$

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where two terms have been added to the expression (7) in order to ensure proper convergence in exceptional cases. The extra terms are usually small and only the third-order Taylor series derivative is converted from the polynomial expression (9). No upper limit is used but the new value is not allowed to increase by more than a factor of 1.4 in order to safeguard the numerical stability. The treatment of the body α is completed by initializing the auxiliary interval, hence $\Delta\tilde{t}_\alpha = \Delta t_\alpha$. A new cycle is entered at Equation (11) which determines the next particle to be considered and the calculations continue as discussed above.

The integration procedure for a high-order scheme using individual time-steps is simple since all decision-making is controlled by the auxiliary variable $\Delta\tilde{t}_i$. It may be noted that the velocity is available only at the end of each interval and proper care must be exercised when evaluating sensitive quantities at a different time as for instance when calculating new integrals of motion. The co-ordinate prediction (12) makes it necessary to preserve all positions at the beginning of each dynamical step. It may also be remarked that the extrapolation of co-ordinates within an interval are not directly useful to the integration since the informations is lost at the next cycle, but this device forms an essential part of the scheme which permits the simultaneous use of widely different time-steps.

A minimum of 28 N storage locations is required by the present method which explicitly includes third-order force differences. It is desirable to make use of extended precision when the computer word contains less than about 10 decimals or if extreme accuracy is intended. In the case of the I.B.M. 360/44 additional precision is used for all co-ordinates and velocities at the beginning of a time-step; $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$, as well as the times t_i and current positions $\mathbf{r}_i$. This requires an additional $10\,N$ storage locations but a 32000 word direct access store would still allow about 600 particles to be studied unless further variables or special treatments are included. The additional time requirement is less than 30% for the same number of integration steps, but the gain in accuracy is considerable when using seven figure precision. Fortunately, more powerful methods are available for treating critical encounters.

The actual choice of the time-step parameter η can only be determined from integration tests, but a value near 2×10^{-4} leads to satisfactory solutions in the absence of extremely close encounters.* A corresponding computing requirement of about one hour per mean crossing time may then be achieved for $N=100$ when the basic addition time is 3.8 μs; similar times for other particle numbers scale as N^2. Alternatively, the time per individual step is given approximately as $1.0\times10^{-3}\,N$ s for $N\gg2$. Nearly all the computing time is accounted for by Equations (5) and (12) together with Equation (11) and the subtraction of the quantity $\Delta\tilde{t}_\alpha$ from all $\Delta\tilde{t}_i$.

The ordinary polynomial method may be used separately or in combination with the regularization treatment discussed below. It is convenient to control the overall integration accuracy by the integrals of motion, in particular the relative error of

* Relative energy errors for a binary with eccentricity 0.92 are then $\Delta E/E = 2\times10^{-5}$ and 7×10^{-6} per revolution, using the two alternative orders of prediction with 234 steps for each component.

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total energy is sensitive to the adopted time-step parameter. An additional and more detailed check of the numerical solutions is provided by the time reversibility of the equations of motion. The ability to deal with close encounters without special treatments may be tested by studying eccentric binary orbits over many revolutions. Accurate solutions are available for a critical three-body case studied by regularization techniques (Szebehely and Peters, 1967); a substantial part of the evolution may also be reproduced reasonably well by the ordinary method.

4. Two-Body Regularization

The Levi-Civita regularization of the plane two-body problem has only recently been generalized to three dimensions where it can be used to study close encounters in stellar dynamics (Kustaanheimo and Stiefel, 1965). It has already been demonstrated that this elegant formulation is extremely efficient in dealing with a variety of three-body configurations (Peters, 1968). In particular, the improvement over ordinary methods becomes apparent in critical two-body encounters since the new equations of motion are non-singular. It is therefore natural to investigate whether this regularization procedure is also effective for the integration of close encounters in larger systems. An extension to large particle numbers requires a suitable formulation of the basic equations of motion as well as the ability to deal with an arbitrary number of two-body encounters at the sam etime. In addition, suitable regularization criteria must be developed in order to combine efficiently the special treatment with the direct method described above.

In the following we make full use of the Hamiltonian formulation of Peters, preserving some of the notation. The four-dimensional equations of motion for the transformed relative co-ordinates $\mathbf{u}$ and momenta $\mathbf{v}$ are given by

$$\mathbf{u}' = \frac{1}{4\mu}\mathbf{v}, \tag{14}$$

$$\mathbf{v}' = 2(E - V)\mathbf{u} + 2\mu R\mathscr{L}^T(\mathbf{F}_k - \mathbf{F}_l), \tag{15}$$

where primes denote differentiation with respect to the fictitious time τ and μ is the reduced mass of the two particles being considered, subsequently to be identified by the individual masses m_k and m_l. The total energy of the system is denoted by E while the perturbing function of the relative motion is given by

$$V = \tfrac{1}{2}(m_k + m_l)\dot{\mathbf{Q}}^2 + \tfrac{1}{2}\sum_{\substack{i=1\\ i\neq k,l}}^{N} m_i\dot{\mathbf{r}}_i^2 - \tfrac{1}{2}\sum_{\substack{i=1\\ j\neq i,k,l}}^{N}\sum_{j=1}^{N} m_i m_j/(|\mathbf{r}_i - \mathbf{r}_j|) \tag{16}$$

which contains the kinetic energy of the centre of mass motion and excludes the contribution $m_k m_l$ from the double summation. The second term of Equation (15) contains the relative Newtonian perturbation

$$\mathbf{F}_k - \mathbf{F}_l = -\sum_{\substack{j=1\\ j\neq k,l}}^{N} m_j\left[\frac{\mathbf{r}_k - \mathbf{r}_j}{|\mathbf{r}_k - \mathbf{r}_j|^3} - \frac{\mathbf{r}_l - \mathbf{r}_j}{|\mathbf{r}_l - \mathbf{r}_j|^3}\right], \tag{17}$$

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and $\mathscr{L}^T$ is the transpose of the generalized Levi-Civita matrix

$$\mathscr{L} = \begin{bmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \end{bmatrix}. \tag{18}$$

Finally, the particle separation R is obtained from the transformed co-ordinates by the relation

$$R = \sum_{j=1}^{4} u_j^2, \tag{19}$$

subsequently written in the form $\mathbf{u}\cdot\mathbf{u}$.

It is readily recognized that an application of Equation (15) to systems with large particle numbers would be prohibitive because of the double summation term in the expression for the perturbing function. Instead we combine the explicit expressions for E and V which simplify to

$$E - V = \frac{1}{2\mu}\mathbf{P}\cdot\mathbf{P} - \frac{m_k m_l}{R}, \tag{20}$$

where $\mathbf{P}$ is the momentum of the relative motion. This relation also follows directly from the regularized Hamiltonian which should be zero (cf. Peters). Thus Equation (20) introduces the binding energy per unit mass of the two-body motion,

$$h = (E - V)/\mu. \tag{21}$$

In order to evaluate Equation (20) when working with regularized quantities we make use of the transformation property

$$\mathbf{P}\cdot\mathbf{P} = \frac{1}{4R}\mathbf{v}\cdot\mathbf{v}. \tag{22}$$

Substituting $\mathbf{u}'$ for $\mathbf{v}$ from Equation (14) and dividing by μ finally gives the desired expression

$$h = [2\,\mathbf{u}'\cdot\mathbf{u}' - (m_k + m_l)]\frac{1}{R}. \tag{23}$$

The relative binding energy per unit mass is obtained at the expense of introducing a division by the particle separation and this procedure does not allow cases to be studied where $R \to 0$. The probability of near collisions, however, is extremely low in simulated clusters and the expression (23) may therefore be used in most calculations of practical interest, instead of the more accurate form (21).

The eight first-order equations of motion (14) and (15) may be combined into four equations of second order for the regularized co-ordinates, giving

$$\mathbf{u}'' = \tfrac{1}{2}h\,\mathbf{u} + \tfrac{1}{2}R\mathscr{L}^T(\mathbf{F}_k - \mathbf{F}_l). \tag{24}$$

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The fictitious time is related to the ordinary integration time t by the regularizing transformation

$$\mathrm{d}t = R\,\mathrm{d}\tau\,. \tag{25}$$

In the present derivation each close pair is treated independently and all fictitious intervals $\Delta\tau$ are converted to ordinary time in order to provide a common frame of reference. This approach differs significantly from that of Peters and allows the introduction of multiple regularizations without affecting the integration of other particles. Such a scheme has many advantages and only requires accurate treatments of the conversion of fictitious time to ordinary time and vice versa.

Actual calculations show that the binding energy formulation leads to a numerical instability in special cases of rapidly varying separations. This difficulty arises because the predicted value of the relative binding energy appears in the equation of motion (24). An analysis of the corresponding unperturbed expression shows that the relative error in binding energy continues to grow if the parameter

$$\varepsilon \simeq \frac{u_0 u_0' \Delta\tau}{u_p^2} \tag{26}$$

exceeds unity. In this first-order derivation which uses the scalar approximation the quantities u_0 and u_0' represent the transformed co-ordinate and velocity at the beginning of the interval $\Delta\tau$, while u_p is the predicted co-ordinate. It is usually sufficient to ensure that the predicted integration step does not violate the adopted stability condition $\varepsilon \lesssim 0.5$, but growing oscillations of the binding energy still appear at extremely small separations. This undesirable behaviour is finally eliminated by using the previously calculated binding energy, rather than the predicted value which is known to one order less accuracy. This procedure is now dynamically consistent for very small perturbations and is only required on rare occasions.

An alternative formulation as yet untried makes it possible to retain the advantage of the binding energy description while avoiding the stability considerations entirely. Thus it has been suggested that an additional equation should be introduced for the binding energy itself (Stiefel, 1967). A convenient expression is obtained for h' by differentiating Equation (23), making use of the equation of motion (24) and the relation $R' = 2\,\mathbf{u}\cdot\mathbf{u}'$, finally giving

$$h' = 2\mathbf{u}'\cdot\mathscr{L}^T(\mathbf{F}_k - \mathbf{F}_l)\,. \tag{27}$$

This equation is completely regular and the right-hand side contains the perturbation term required by the equation of motion (24). Again the new binding energy must be obtained by prediction but the perturbation contribution remains well behaved for small separations as in the classical expression $\dot{h} = \dot{\mathbf{R}}\cdot(\mathbf{F}_k - \mathbf{F}_l)$. In addition it may be noted that the procedure of integrating the binding energy separately gains one order of accuracy compared to Equation (23) which involves the regularized velocity. The subsequent discussion therefore assumes the integration treatment based on Equation (27) where the initial value is given by Equation (23).

5. Transformations

Assuming that the pair m_k, m_l, has been selected for special treatment, we introduce the relative co-ordinates and momenta*

$$\mathbf{R} = \mathbf{r}_k - \mathbf{r}_l, \tag{28}$$

$$\mathbf{P} = \mu(\dot{\mathbf{r}}_k - \dot{\mathbf{r}}_l). \tag{29}$$

The transformation to regularized co-ordinates takes two forms depending on the sign of the first component of the separation vector (X, Y, Z). Thus for $X>0$ the initial components of the four-vector $\mathbf{u}$ are given by

$$\begin{aligned} u_1 &= [\tfrac{1}{2}(R + X)]^{1/2}, \\ u_2 &= Y/2u_1, \\ u_3 &= Z/2u_1, \\ u_4 &= 0, \end{aligned} \tag{30}$$

while for $X<0$ the proper choice is

$$\begin{aligned} u_2 &= [\tfrac{1}{2}(R - X)]^{1/2}, \\ u_1 &= Y/2u_2, \\ u_3 &= 0, \\ u_4 &= Z/2u_2. \end{aligned} \tag{31}$$

In both cases the inverse relations are

$$\begin{aligned} X &= u_1^2 - u_2^2 - u_3^3 + u_4^2 \\ Y &= 2(u_1u_2 - u_3u_4) \\ Z &= 2(u_1u_3 + u_2u_4). \end{aligned} \tag{32}$$

It can readily be seen that Equation (32) implies the relation (19).

The regularized momentum vector $\mathbf{v}$ is transformed according to

$$\mathbf{v} = 2\mathscr{L}^T\mathbf{P}, \tag{33}$$

where the transpose matrix is given by

$$\mathscr{L}^T = \begin{bmatrix} u_1 & u_2 & u_3 \\ -u_2 & u_1 & u_4 \\ -u_3 & -u_4 & u_1 \\ u_4 & -u_3 & u_2 \end{bmatrix}. \tag{34}$$

The relation (33) implies the non-holonomic condition

$$u_4v_1 - u_3v_2 + u_2v_3 - u_1v_4 = 0. \tag{35}$$

* The definition of relative co-ordinates and momenta used by Peters should be reversed in order to be consistent with the final equation of motion. A correct derivation is given in the original Ph.D. thesis, Yale University, 1968.

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The integration accuracy can be checked using Equations (27) or (35). In practice it is more convenient to work with $\mathbf{u}$ and $\mathbf{u}'$ where the latter is defined by Equation (14). The equation of motion (24) then plays the role of Equation (5) and we can make use of the polynomial method discussed above for the integration.

The complete solution of the regularized motion is obtained by introducing the centre of mass co-ordinates

$$\mathbf{Q} = \frac{m_k \mathbf{r}_k + m_l \mathbf{r}_l}{m_k + m_l}, \tag{36}$$

with the corresponding equation of motion

$$\ddot{\mathbf{Q}} = \frac{m_k \mathbf{F}_k + m_l \mathbf{F}_l}{m_k + m_l}. \tag{37}$$

It may be noted that only the two perturbations enter in the centre of mass acceleration since the dominant terms cancel analytically. The proposed two-body regularization procedure requires in all 16 equations as compared to 12 equations for the ordinary method. Even so there is no loss of efficiency since the perturbation calculation is by far the most time-consuming for large particle numbers. The longer intervals permitted by the regularized solution therefore represent a net gain over standard integration schemes.

The original quantities may be obtained at any time from the transformations

$$\begin{aligned}
\mathbf{R} &= \mathscr{L} u, \\
R &= \mathbf{u} \cdot \mathbf{u}, \\
\mathbf{P} &= 2\mu \mathscr{L} \mathbf{u}'/R, \\
\mathbf{r}_k &= \mathbf{Q} + \mu \mathbf{R}/m_k, \\
\mathbf{r}_l &= \mathbf{Q} - \mu \mathbf{R}/m_l, \\
\dot{\mathbf{r}}_k &= \dot{\mathbf{Q}} + \mathbf{P}/m_k, \\
\dot{\mathbf{r}}_l &= \dot{\mathbf{Q}} - \mathbf{P}/m_l,
\end{aligned} \tag{38}$$

with the reduced mass

$$\mu = \frac{m_k m_l}{m_k + m_l}. \tag{39}$$

The present integration procedure requires an accurate determination of the ordinary time corresponding to a fictitious time-step. Several methods may be used for the conversion of regularized time; here we make use of the Taylor series expansion

$$\Delta t = t_0' \, \Delta\tau + \tfrac{1}{2} t_0'' \, \Delta\tau^2 + \tfrac{1}{6} t_0''' \, \Delta\tau^3 + \tfrac{1}{24} t_0^{(\mathrm{IV})} \, \Delta\tau^4 + \tfrac{1}{120} t_0^{(\mathrm{V})} \, \Delta\tau^5. \tag{40}$$

The desired coefficients evaluated at the beginning of the interval $\Delta\tau$ are readily obtained by successive differentiations of the second Equation (38) with respect to

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the fictitious time, using the definition (25). The first three terms are given by

$$\begin{aligned} t_0' &= \mathbf{u}\cdot\mathbf{u}, \\ t_0'' &= 2\mathbf{u}'\cdot\mathbf{u}, \\ t_0''' &= 2\mathbf{u}''\cdot\mathbf{u} + 2\mathbf{u}'\cdot\mathbf{u}'. \end{aligned} \tag{41}$$

All derivatives of $\mathbf{u}$ required by Equation (40) are known from the high-order integration scheme, hence the conversion to ordinary time is very efficient. It may be noted that the regularized polynomial derivatives should be converted to actual Taylor series derivatives at the time τ_0 by the equivalent procedure of Equation (9). Numerical tests show that the adopted expansion converges rapidly since all the terms are well behaved.

An inverse relation is also required for extrapolation within an interval $\Delta\tau$ in order to transform the regularized co-ordinates at times not coinciding with the end-points. In this case less accuracy is needed and we adopt the expansion

$$\Delta\tilde{\tau} = \dot{t}_0\,\Delta t + \tfrac{1}{2}\ddot{t}_0\,\Delta t^2 + \tfrac{1}{6}\dddot{t}_0\,\Delta t^3, \tag{42}$$

using the definition (25),

$$\dot{t}_0 = 1/R. \tag{43}$$

The two higher derivatives can be expressed in terms of the quantities (41) as

$$\begin{aligned} \ddot{t}_0 &= -\frac{t_0''}{R^3}, \\ \dddot{t}_0 &= \left[\frac{3t_0''^2}{R} - t_0'''\right]\frac{1}{R^4}. \end{aligned} \tag{44}$$

The division by small values of R may be permitted since it does not effect the integration of the relative motion. Thus the procedure (42) is only required for the purpose of calculating $\ddot{\mathbf{Q}}$ or $\ddot{\mathbf{r}}_i$; the former may just as well be evaluated at the nearest end-point, while it is dynamically consistent to use the centre of mass approximation for very small separations when computing the force contribution to other particles.

The regularized components are also integrated by the fourth-order polynomial method since the acceleration calculations are still time-consuming. The formulation described by Equations (6)–(10) may be used to obtain a consistent starting procedure for the centre of mass motion. Coefficients representing polynomial derivatives are first determined for each component, excluding the dominant contribution, and the desired expressions are combined in the manner of Equation (37). The centre of mass co-ordinates and velocities are initialized and the integration proceeds as in the ordinary method, except that the co-ordinate transformation (38) must be performed in order to calculate the acceleration (37).

It is not possible to make use of the explicit starting scheme for the relative motion, however. Instead a fitting procedure is employed for obtaining Taylor series derivatives which are then converted in the usual manner. Denoting the regularized acceleration

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at time τ_0 by $\mathbf{G}_0$ instead of $\mathbf{u}''$, we write an expansion in terms of $\tau_r = \tau - \tau_0$ as

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0'\tau_r + \tfrac{1}{2}\mathbf{G}_0''\tau_r^2 + \tfrac{1}{6}\mathbf{G}_0'''\tau_r^3 . \tag{45}$$

Successive accelerations $\mathbf{G}_j$, $j=1, 2, 3$ are determined from Equation (24) at three equal intervals $\delta\tau$ by advancing all co-ordinates appropriately, including the centre of mass. The fitting intervals $\delta\tau$ are chosen such that $3\delta\tau = 0.5\Delta\tau_0$, where $\Delta\tau_0$ is the initial time-step to be used by the high-order integration. The resulting coefficients are given by

$$\begin{aligned}
\mathbf{G}_0' &= \left[-\tfrac{11}{6}\mathbf{G}_0 + 3\mathbf{G}_1 - \tfrac{3}{2}\mathbf{G}_2 + \tfrac{1}{3}G_3\right]\frac{1}{\delta\tau}, \\
\mathbf{G}_0'' &= \left[\mathbf{G}_0 - \tfrac{5}{2}\mathbf{G}_1 + 2\mathbf{G}_2 - \tfrac{1}{2}\mathbf{G}_3\right]\frac{1}{\delta\tau^2}, \\
\mathbf{G}_0''' &= \left[-\tfrac{1}{6}\mathbf{G}_0 + \tfrac{1}{2}\mathbf{G}_1 - \tfrac{1}{2}\mathbf{G}_2 + \tfrac{1}{6}\mathbf{G}_3\right]\frac{1}{\delta\tau^3}.
\end{aligned} \tag{46}$$

Finally, the conversion to polynomial derivatives is performed in analogy with the procedure of Equations (8) and (9) and the regularized integration may be continued by the usual method. Starting coefficients for the right-hand side of Equation (27) are determined in a similar manner, writing Equation (45) as an expansion for the function $H \equiv h'$. Subsequent values of the binding energy are then obtained by integrating the corresponding polynomial once.

6. Regularization Parameters

Close encounters between ordinary particles lead to a shortening of the corresponding time-steps which is essentially independent of the relative binding energy for small separations. It is therefore natural to specify a critical interval $\Delta t_{\min}$ and a corresponding separation $R_{\min}$ to be used as an indication of suitable cases for special treatment. Once a particle m_k satisfies the condition $\Delta t_k < \Delta t_{\min}$ and the time-step is decreasing, a search is made for the body m_l which contributes the greatest force component, at the same time noting all other particles j inside a somewhat larger separation, say, $3R_{\min}$. The pair m_k, m_l is accepted for regularization, provided that $R < R_{\min}$ and the relative force is dominant. The latter requirement implies that

$$\frac{m_k + m_l}{|\mathbf{r}_k - \mathbf{r}_l|^2} > \frac{m_l + m_j}{|\mathbf{r}_l - \mathbf{r}_j|^2} \tag{47}$$

for all j, k, l. The condition (47) allows for the possibility of body m_k being close to another regularized pair. It is also prudent to include approaching particles only in view of the additional calculations for the starting procedure.

The special treatment may be terminated in several ways, depending on the circumstances. It is convenient to make use of the invariant two-body perturbation

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defined by

$$\gamma = \frac{|\mathbf{F}_k - \mathbf{F}_l| \, R^2}{m_k + m_l}. \tag{48}$$

The latter quantity is particularly useful for deciding when to end the regularization of close binaries. Thus it is natural to replace the components m_k, m_l by, say, the pair m_l, m_j when the latter particle gives rise to the perturbation $\gamma \gtrsim 1$ since the original binary motion is then no longer dominant.

Regularization of hyperbolic cases or wide binaries is normally terminated by the combined criterion

$$R > R_0, \quad \gamma > \gamma_{\max}, \tag{49}$$

where R_0 denotes the initial separation. The second condition (49) makes it possible to continue the special treatment outside the initial separation; this feature is particularly useful for hyperbolic orbits with $R_0 \ll R_{\min}$, or when dealing with eccentric binaries where the apocentre distance exceeds the critical value $R_{\min}$. The regularization criteria discussed above are completely general; consistent values may be chosen from trial integrations or invariant definitions of close encounters.

The integration interval for regularized binary motion may be determined by reference to the orbital period. Bearing in mind the form of the equation of motion and the time transformation (25), we adopt an expression of constant time-step modified by perturbations,

$$\Delta\tau = \frac{2\pi}{\mathcal{N}} \left[\frac{1}{2|h|} \right]^{1/2} \frac{1}{(1 + 1000\,\gamma)^{1/3}}, \tag{50}$$

where the parameter $\mathcal{N}$ denotes the number of integration steps during one unperturbed revolution. The correction term is usually small but allows for a significant reduction of step-size in the presence of strong perturbations which lead to rapid variations of the binding energy.

Equation (50) is equally suitable for treating hyperbolic motion. The precaution is taken of replacing the unperturbed part of the predicted time-step by a constant β in all cases which would otherwise give $\Delta\tau > \beta$ in the absence of perturbations. An additional safety measure is included by using half the predicted value of the initial step $\Delta\tau_0$; subsequent intervals are allowed to increase by a factor of 1.2. The adopted time-step definition is not unique and alternative expressions may therefore be tried. It may be noted that the period of the regularized equation of motion (24) corresponds to twice the Keplerian value. This fundamental property of the Kustaanheimo-Stiefel transformation demonstrates clearly the effectiveness of the method.

Direct calculations of close binary orbits are also time-consuming when using the regularization description. In such cases the number of binary revolutions per crossing time may be very large, while the corresponding perturbation is often sufficiently small to be neglected (Aarseth, 1970). The simplification of unperturbed motion may also be introduced here since the Keplerian period is known in ordinary

time units. Instead we reduce the number of interacting bodies to include the nearest neighbours which contribute the main part of the fluctuating force field. Thus the effect of distant particles tends to cancel when the relative motion is integrated over one complete revolution. Furthermore, it is only by replacing the variables $\mathbf{r}_k$, $\mathbf{r}_l$ by the set $\mathbf{Q}$, $\mathbf{R}$ that this technique can be used advantageously since the total centre of mass acceleration is usually required much less frequently.

The perturbation is included from all particles i which satisfy the condition

$$\frac{m_i}{|\mathbf{Q}-\mathbf{r}_i|^3} \gtrsim \frac{1}{\kappa^3 R^3}, \tag{51}$$

where κR represents the limiting separation for bodies of mean mass unity. Conversely, the force contribution to ordinary particles may be calculated by the centre of mass approximation when the distance to regularized pairs exceeds κR. It may be noted that the adopted expression is consistent with the tidal limit approximation of the perturbation (48) and corresponds to $\gamma \simeq \kappa^{-3}$, neglecting the mass dependence. The list of neighbours is updated at every apocentre passage as determined from the change in sign of the radial velocity R'.

Numerical values of the regularization parameters have not been discussed above since the choice is to some extent arbitary and depends on the desired integration accuracy. One example with eccentricity 0.7 shows that $\mathcal{N}=50$ is sufficient to keep the relative binding energy error per revolution below 1×10^{-6}, while $\mathcal{N}=63$ improves the accuracy to 3×10^{-7}, when all calculations are performed in extended precision. The adopted parameters for the first large N-body integration using regularization are given for completeness; i.e., $\Delta t_{\min}=1\times10^{-5}$, $R_{\min}=0.01$, $\gamma_{\max}=0.01$, $\mathcal{N}=50$, $\beta=0.01$, $\kappa=100$ for one case $N=500$, employing the energy scaling $E=-\frac{1}{4}N^2$ with mass units $\sum m_i=N$. The fast perturbation calculation is only used for close binaries satisfying the condition $h<-N$, but this procedure would be equally consistent for all regularizations. Finally, we remark that the additional transformations required when treating other particles inside the distance κR partly offsets the advantages of regularizing large separations, hence the conservative choice of the first three parameters.

7. Special Considerations

It is essential to organize tables of variables in a systematic way in order to facilitate the simultaneous treatment of ordinary particles and regularized pairs. For convenience we distinguish between global quantities g_i such as $\mathbf{r}_i$, $\dot{\mathbf{r}}_i$, etc. and regularized variables ρ_j denoting $\mathbf{u}$, $\mathbf{u}'$. The sequential arrays $\{g_i\}$ are modified to include the regularized components first. The last member of a global particle array is then g_N as usual but the centre of mass corresponding to the first regularization is added as g_{N+1}. The extension to an arbitrary number of regularized pairs follows quite naturally in the present treatment. Thus an alteration to the existing situation is performed by moving all relevant quantities up or down in the tables and deleting or adding the corresponding centre of mass.

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Consider a general situation with n separate close pairs. The particle arrays $\{g_i\}$ where $i \leqslant 2n$ then represent the transformed components with corresponding relative parameters $\{\rho_j\}$, $j \leqslant n$. Subsequent locations $2n+1$, ..., N are assigned to ordinary particles, followed by the centre of mass arrays $\{g_{N+j}\}$ with $j \leqslant n$. It is therefore quite simple to distinguish between the different procedures required by the three cases $\alpha \leqslant 2n$, $2n < \alpha \leqslant N$, $\alpha > N$, where α is determined by Equation (11). In addition, co-ordinate predictions and force calculations are more efficient when similar quantities are stored sequentially.

Regularization treatments are terminated by the transformations (38) after which the component co-ordinates and velocities are restored to the original locations. At the same time any quantities g_{N+j} and ρ_j introduced more recently are updated consistently. Finally, the starting procedure described by Equations (5)–(10) is applied to each component and the integration proceeds normally. A minimum of reorganization is achieved by arranging all arrays $\{g_i\}$ in terms of decreasing mass initially since heavy bodies are most frequently involved in close encounters. It is then numerically advantageous to perform the force summation (5) in reverse order.

In conclusion, it may be emphasized that a considerable programming effort is required in order to make efficient use of the methods described above. At the same time the introduction of two-body regularization represents a significant improvement of technique which permits more critical configurations to be studied. Some efficiency is lost, however, when integrating multiple close encounters if there are no dominant pairs which may be selected for regularization. An alternative treatment is available for such cases (Heggie, 1972) but the introduction of a third procedure has not yet been attempted. Further programming details are available upon request*.

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* The treatment based on Equation (27) has now been adopted. Energy errors for a binary with eccentricity 0.92 then improve from $\Delta E/E = -5 \times 10^{-6}$ to -8×10^{-8} per revolution, if $\mathcal{N} = 50$.