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Simulation of Binary-Single Star and Binary-Binary Scattering

M. E. ALEXANDER

Institute of Computer Science and Department of Physics, University of Guelph, Guelph, Ontario, N1G 2W1 Canada

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Numerical methods for integrating gravitational 3- and 4-body systems are investigated and tested. The methods employ multiple-pair regularization schemes for N-body systems proposed by Aarseth, Zare, and Heggie, which use the Kustaanheimo–Stiefel transformation for regularizing 2-body collisions, in conjunction with a number of different time transformations between "physical" and "parameter" time. These transformations can be chosen so as to make the singularity in the equations of motion, caused by many-body collisions, as mild as possible. The various time transformations are tested on both 3- and 4-body systems by comparing the numerical with known analytical solutions, and by time reversal of the integrations through many-body close encounters. In addition, the technique of Zare and Szebehely for stabilizing numerical integrations is investigated for each of the time transformations. It is found that when the time transformation is a function of the interparticle separations only, stabilization leads to a significant improvement in performance for those transformations in which the singularity occuring due to many-body collisions is strong (algebraic), but has no decisive effect when the singularity has been softened by an optimal choice of transformation. The most satisfactory time transformation appears to be one involving the Lagrangian, together with the regularization scheme proposed by Aarseth and Zare.

Computer programs for binary-single star and binary-binary scattering have been developed and are described. They can be used in an extensive project for determining scattering cross sections with any of the above methods. They are used here to compare the performance of these methods, for a fixed set of intial conditions, on scattering involving "hard" binaries, in which strong resonances can occur. It is found that the outcome of the scattering, for example, the identity of the escaping particle(s), can vary with method, thus reflecting the inherent instability of the N-body problem.

1. INTRODUCTION

Numerical integrations of the gravitational N-body problem, for simulating the evolution of star clusters, have established the important dynamical role of binaries formed primordially or as a result of 3-body interactions. Cluster evolution leads to high central densities which favour the formation of binary and multiple subsystems. As a result of encounters with other stars, the binary may subsequently be disrupted, increase its binding energy, or even exchange one of its components with the passing star. If the binding energy of the binary increases as a result of the scattering, the escaping star gains energy which may then be imparted to the other

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members of the cluster, or may lead to the escape of the star from the cluster altogether.

The cross sections and reaction rates associated with binary-single star scattering have been determined in two ways. An approximate analytic theory has been developed by Heggie [11] which, because of its generality, has been of considerable value as a starting point for computer calculations of cluster evolution (Spitzer and Mathieu [30]; Retterer [28]). Detailed numerical integrations of many thousands of scattering events have been carried out by Saslaw, Valtonen, and Aarseth [29], Hills [12], and several others since, most notably by Hut and Bahcall [14] (with references to earlier work) and Hut [15]. These numerical results provide a statistical description of binary-single star scattering in terms of parameters such as the size and eccentricity of the initial and final binary orbits, and kinetic energies of incoming and escaping stars.

Binary-binary scattering is likely to be even more frequent than binary-single star scattering in the late stages of collapse of a cluster already containing an appreciable fraction of binaries. Due to their greater mass than single stars, binaries congregate in the dense core of the cluster. An approximate asymptotic theory, based on Heggie's analysis of binary-single star scattering [11], was developed by Spitzer and Mathieu [30], but they are forced to assume that the binary orbits before scattering are of very different size. On the numerical side, some scattering experiments have been carried out by various investigators [29, 9, 13]. Recently Mikkola [21–25] has developed a sophisticated program for performing several thousand scattering experiments to obtain cross sections and reaction rates, thereby providing a statistical description analogous to the binary-single star case mentioned above. The numerical integrations are more time-consuming than for binary-single star scattering, and several more outcomes are possible.

A fundamental difficulty associated with numerical work is the occurence of resonance scattering, in which the incoming star or binary is captured and an unstable triple system formed. Resonance scattering is most common when the kinetic energy of the incoming star is less than the binding energy of the binary (the binary is then referred to as being "hard"). The triple system may survive for an indefinitely long time before breaking up into a binary plus escaping star. Furthermore, the triple system may execute complicated orbits which may result in several very close encounters between the members. The occurence of the $1/r^2$ singularity in the gravitational force can lead to loss of numerical accuracy or stability, unless suitably small step-sizes are chosen: this may lead to excessively large numbers of steps when integrating an orbit. Several regularization techniques have been proposed to remove this singularity and provide equations which are regular with respect to collisions between pairs of particles [5, 10, 35]. Two-body regularization techniques using the Kustaanheimo–Stiefel (KS) transformation [16] have been very successful in overcoming these numerical difficulties [1–3, 27].

In view of the difficulties associated with multiple close encounters occuring during resonance scattering (in both 3- and 4-body systems), a regularizing transformation is desirable. The aim of this paper is to examine a number of time-

smoothing techniques and regularization, based on the KS-transformation, for 3- and 4-body systems, and to compare them as to efficiency and accuracy in numerical integration. These methods will also be compared with methods employing the classical equations of motion with the $1/r^2$ singularity [14, 15, 37]. In Section 2, a number of regularizing transformations are proposed, based on the multiple pair-regularization methods developed by Aarseth and Zare [5], Zare [35], and Heggie [10]. Section 3 describes numerical testing procedures, involving time-reversal tests on critical encounters and comparison with known analytic (periodic) solutions. The results of numerical tests, for both 3- and 4-body systems and for a large class of methods, are also presented in this section. In Section 4, a general computer program, similar to Mikkola's [21], is described for carrying out extensive binary-single star and binary-binary scattering, in which the initial conditions for scattering are automatically generated in the program by random sampling from the appropriate distributions. The procedure for terminating a particular orbit calculation is also described. The various proposals for regularization and time-smoothing are easily inserted into this program. The performance of these methods applied to a particular set of scattering initial conditions is compared. Finally, some recommendations are made as to the best method for use in generating a large sample of data for obtaining scattering cross sections and reaction rates for binary-single star and binary-binary scattering.

2. Regularization

Numerical experiments on N-body systems have shown that close encounters between particles lead to a serious loss of accuracy of the solutions, as a direct result of the $1/r^2$ singularity in the inter particle force. The goal of regularization is to remove this singularity in the equations by a transformation of the co-ordinates followed by a time transformation to a new "regularized" time s. For motion in the (x, x_2) plane, Levi-Civita [18] proposed the parameter representation $w = Q_1 + iQ_2$ which maps onto the physical plane $z = x_1 + ix_2$ by the conformal transformation $z = w^2$. This may be written as

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = L(Q) \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}$$

where

$$L(Q) = \begin{pmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{pmatrix}$$

is an orthogonal matrix with row/column norm $Q_1^2 + Q_2^2 = \sqrt{x_1^2 + x_2^2} = R$. There is no corresponding transformation for 3 dimensions involving only 3 parameters

(Q_1, Q_2, Q_3); however, Kustaanheimo and Stiefel [16] were able to find a 4-dimensional representation (Q_1, Q_2, Q_3, Q_4)

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ 0 \end{pmatrix} = L(Q) \begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{pmatrix} \tag{2.1}$$

where $L(Q)$ is the orthogonal matrix

$$L(Q) = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{pmatrix} \tag{2.2}$$

with row/column norm

$$\begin{aligned} Q_1^2 + Q_2^2 + Q_3^2 + {}^2_4 &= \sqrt{x_1^2 + x_2^2 + x_3^2} \\ &= R. \end{aligned} \tag{2.3}$$

Furthermore the physical momentum (p_1, p_2, p_3) may be transformed to the 4-dimensional representation

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ 0 \end{pmatrix} = \frac{1}{2R} L^T(Q) \begin{pmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \end{pmatrix} \tag{2.4}$$

where the fourth component of the right-hand side represents a constant of motion which may be chosen to be zero [16]. In keeping with previous notation [5, 10, 35], we denote the 3-vectors with non-zero components on the left-hand sides of Eqs. (2.1) and (2.4) by $\mathbf{q}$ and $\mathbf{p}$, respectively; similarly, their 4-vector regularized representations are denoted by $\mathbf{Q}$ and $\mathbf{P}$. We may thus discard the fourth row of the matrix L; the resulting 3 by 4 matrix is the same as $\frac{1}{2}A^T(\boldsymbol{Q})$ in [5, 10, 35].

The KS-transformation forms the basis of the regularization techniques of Aarseth, Zare, and Heggie for arbitrary 2-body collisions in N-body systems. They may be derived by canonical transformations of the dynamical variables $\mathbf{q}_{ij}$ and $\mathbf{p}_{ij}$, representing the position vector separating a pair of particles (i, j) and its conjugate momentum, respectively, in which the KS-transformation (Eqs. (2.1) and (2.4)) appears as one of the canonical transformations. The index ij can range over all $N(N-1)/2$ possible pairs of particles, as in Heggie's global scheme, or over a subset of $k < N(N-1)/2$ pairs, as in the Aarseth–Zare scheme, in which one of the par-

ticles is chosen as a reference body and regularization of its collision with k other particles is performed.

Before the KS-transformation can be applied, the particle separations and their conjugate momenta in physical 3-space must be specified as dynamical variables for the system. This involves one or more canonical transformations of the variables $(\mathbf{q}_i', \mathbf{p}_i')$ where $\mathbf{q}_i'$ is the Cartesian co-ordinate vector of the ith particle in some inertial frame of reference and $\mathbf{p}_i'$ its conjugate momentum. The corresponding Hamiltonian (in the centre-of-mass frame) is given by

$$H' = \sum_{i=1}^{N} \frac{(p_i')^2}{2m_i} - \sum\sum_{i<j} \frac{m_i m_j}{R_{ij}} \tag{2.5}$$

where $R_{ij} = |\mathbf{q}_i' - \mathbf{q}_j'|$. In Aarseth and Zare's schemes, $\mathbf{q}_N'$ becomes an ignorable co-ordinate and $\mathbf{p}_N = 0$. In the new variables, $\mathbf{q}_i$ represents the separation of particle i from particle N, $1 \leqslant i < N$. Also, k was chosen to be $(N-1)$, so that the separation vectors between the reference body and each of the remaining $(N-1)$ particles was regularized. The new Hamiltonian is then given by

$$H = \sum_{i=1}^{N-1} \frac{p_i^2}{2\mu_i} + \frac{1}{m_N} \sum\sum_{i<j\leqslant N-1} \mathbf{p}_i^T \mathbf{p}_j - m_N \sum_{i=1}^{N-1} \frac{m_i}{R_{iN}} - \sum\sum_{i<j\leqslant N-1} \frac{m_i m_j}{R_{ij}} \tag{2.6}$$

where $\mu_i \equiv m_i m_N/(m_i + m_N)$, and $\mathbf{p}_i = \mathbf{p}_i'$.

In Heggie's scheme, if $N > 3$ then the total number of separation vectors exceeds the number of particles, so that the $\mathbf{q}_{ij}$ are not independent. Heggie has given a method for enlarging the dynamical system to accommodate the $\mathbf{q}_{ij}$ as dynamical variables and obtain their conjugate momenta. From a practical point of view, the advantage of this scheme is that all particles are treated on an equal basis, unlike the Aarseth–Zare scheme in which it is necessary to change the reference body in the course of the integrations so as to regularize an appropriate subset of k inter-particle separations at each stage. Its disadvantage is that the number of equations is $O(N^2)$ instead of $O(N)$ as in the Aarseth-Zare scheme. More specifically, Zare's method for regularization of k particle separations involves $2(3N-3+k)$ equations, whereas Heggie's requires $4N(N-1)$ equations (excluding one for the time transformation). The cases $N=3$ and $N=4$ are of particular interest, for binary-single star and binary-binary scattering, respectively, and N is small enough that the two approaches may still be competitive with regard to efficiency of computation.

Thus far, the transformation of physical time has not been specified. For the simple 2-body case it is given by

$$\frac{dt}{ds} = R \tag{2.7}$$

where R is the separation. Thus, s plays the role of the eccentric anomaly in Keplerian orbital motion. For an N-body system, consider the more general transformation

$$\frac{dt}{ds} = g(\mathbf{q}, \mathbf{p}). \tag{2.8}$$

The Hamiltonian in the extended phase space $(\mathbf{q}, t, \mathbf{p}, h)$ is

$$\Gamma = H(\mathbf{q}, \mathbf{p}) - h$$

where h is the (constant) energy along a particular orbit and $(-h)$ is conjugate to the co-ordinate t. The corresponding Hamiltonian in regularized phase space is

$$\Gamma^*(\mathbf{Q}, t, \mathbf{P}, h) = g\Gamma = g[H(\mathbf{q}(\mathbf{Q}), \mathbf{p}(\mathbf{Q}, \mathbf{P})) - h] \tag{2.9}$$

and the canonical equations of motion are

$$\frac{d\mathbf{Q}_{ij}}{ds} = \frac{\partial \Gamma^*}{\partial \mathbf{P}_{ij}} \tag{2.10}$$

$$\frac{d\mathbf{P}_{ij}}{ds} = -\frac{\partial \Gamma^*}{\partial \mathbf{Q}_{ij}} \tag{2.11}$$

$$\frac{dt}{ds} = \frac{\partial \Gamma^*}{\partial(-h)} = g. \tag{2.12}$$

In order to remove the singularity in (2.10) and (2.11) caused by the collision of particles i and j, and to ensure that s remains finite as t approaches a finite limit as $R_{ij} \to 0$, the only allowed possibility is that $g \sim R_{ij}$ as $R_{ij} \to 0$ [6, 32]. Thus, a possible choice for a time transformation is

$$g = \prod_{i<j} R_{ij} \tag{2.13}$$

[10, 35]. However, we shall consider the general case given by Eq. (2.8), in which $\mathbf{q}$ and $\mathbf{p}$ are related by the KS-transformation (2.1)–(2.4) to the regularized variables $\mathbf{Q}$ and $\mathbf{P}$. Although one cannot regularize triple or higher-order collisions, it may still be possible to choose g in such a way as to make the singularity caused by the simultaneous collision of more than two bodies as "smooth" as possible. By this reasoning, one hopes to make the numerical integrations through a multiple close encounter as accurate and efficient as possible. Such an approach was employed by Heggie [10] for 3-body systems, and was shown to yield better numerical results than the "less optimal" transformation (2.13).

During approach to a collision, at time t_c, of any pair of particles a distance $R(t)$

apart, we have that $R \sim (t_c - t)^{2/3}$ (see, for example, [19]). Hence, in general, near a multiple collision, we have

$$\begin{aligned} \mathbf{q}_{ij} &\sim (t_c - t)^{2/3} \\ \mathbf{p}_{ij} &\sim (t_c - t)^{-1/3} \end{aligned} \tag{2.14}$$

and

$$H(\mathbf{q}, \mathbf{p}) \sim (t_c - t)^{-2/3}. \tag{2.15}$$

Now suppose that $dt/ds = g \sim (t_c - t)^{\alpha}$; then, using Eqs. (2.1)–(2.4) and (2.9)–(2.12) we derive

$$\frac{d\mathbf{q}_{ij}}{ds} \sim (t_c - t)^{\alpha - 1/3}; \qquad \frac{d\mathbf{p}_{ij}}{ds} \sim (t_c - t)^{\alpha - 4/3} \tag{2.16}$$

and

$$\frac{d\mathbf{Q}_{ij}}{ds} \sim (t_c - t)^{\alpha - 2/3}; \qquad \frac{d\mathbf{P}_{ij}}{ds} \sim (t_c - t)^{\alpha - 1} \tag{2.17}$$

where s and t are related by

$$(t_c - t) \sim (s_c - s)^{1/(1-\alpha)} \qquad (\alpha \neq 1) \tag{2.18}$$

or

$$(t_c - t) \sim e^{-Cs} \qquad (\alpha = 1;\ C = \text{const} > 0). \tag{2.19}$$

By an appropriate choice of α, we may ensure that some, but *not all*, of the Eqs. (2.16)–(2.19) remain regular as $t \to t_c^-$. The same conclusion applies when considering $t > t_c$.

The straightforward choice for g, given by Eq. (2.13), regularizes 2-body collisions, but still leads to badly behaved singularities in higher-order collisions. For triple collisions in a 3-body system, Heggie proposed the transformation

$$g = \frac{R_{12} R_{23} R_{13}}{(R_{12} + R_{23} + R_{13})^{3/2}} \tag{2.20}$$

which corresponds to $\alpha = 1$ (since $R_{ij} \sim (t_c - t)^{2/3}$). Thus, Eqs. (2.17) remain regular; however, Eq. (2.19) indicates that $s \to \infty$ at collision. A generalization of (2.20) for simultaneous collisions of n bodies in an N-body system ($n \leqslant N$)

$$g = \frac{\prod_{i<j} R_{ij}}{(\sum_{i<j} R_{ij})^{\beta}} \tag{2.21}$$

would likewise impose the choice $\beta = n(n-1)/2 - \frac{3}{2}$. Note that this applies only to the Heggie scheme: for the Aarseth–Zare scheme, for which $\mathbf{q}_{iN}$ $(1 \leqslant i < N-1)$ are generalized coordinates, we must choose

$$g = \frac{\prod_{i=1}^{n} R_{iN}}{(\sum_{i=1}^{n} R_{iN})^{\beta}} \tag{2.22}$$

with $\beta = n - \frac{3}{2}$. This transformation was used by Aarseth [4] for the special case of triple collisions in a 3-body system ($n = 2$, $\beta = \frac{1}{2}$). If $n < N$, then more than one subsystem can undergo a multiple (n-fold) collision, and in each case the choice of g must be invariant to re-labelling of the particles. Thus, for 4-body systems, possible transformations are

Heggie's scheme:

(i) Triple collisions

$$g = R_{12}R_{13}R_{14}R_{23}R_{24}R_{34}\left[\frac{1}{R_{23}+R_{24}+R_{34}} + \frac{1}{R_{13}+R_{14}+R_{34}} + \frac{1}{R_{12}+R_{14}+R_{24}} + \frac{1}{R_{12}+R_{13}+R_{23}}\right]^{3/2} \tag{2.23}$$

(ii) Quadruple collisions

$$g = R_{12}R_{13}R_{14}R_{23}R_{24}R_{34}/(R_{12}+R_{13}+R_{14}+R_{23}+R_{24}+R_{34})^{9/2} \tag{2.24}$$

Aarseth–Zare scheme (reference body labelled "4"):

(iii) $$g = R_{14}R_{24}R_{34}/(R_{14}+R_{24}+R_{34})^{3/2}. \tag{2.25}$$

It should be noted that, in the Aarseth-Zare scheme, the interparticle separations $\mathbf{q}_{ij} (i \neq N, j \neq N)$ are *not* regularized. This suggests the following strategy for choosing the reference body in the course of numerical integration of Eqs. (2.10)–(2.12): find the minimum distance of separation among $N(N-1)/2$ pairs of particles, and choose the reference body to be one of the particles defining this minimum separation. In the numerical results described in this paper, the reference body was chosen to be the particle having the smaller index in the original labelling scheme for the particles. A more sophisticated algorithm for resolving the ambiguity according to additional criteria would have entailed more frequent changes in reference body and re-initialization of the regularization variables $(\mathbf{Q}_{iN}, \mathbf{P}_{iN})$, which was felt to be unwarranted.

Another transformation, also involving only the R_{ij}'s, has been discussed many times before (for example, [6, 35]):

$$g = 1/F \tag{2.26}$$

in which F is related to the potential energy function of the system, U, by $U = -F$ ($F > 0$). This transformation has the advantage of possessing a first integral

$$t = \frac{1}{2h}\left[\sum_{i=1}^{N} (\mathbf{p}_i')^T \mathbf{q}_i' - s\right] + \text{constant} \tag{2.27}$$

so that Eq. (2.12) for dt/ds need not be integrated.

In considering the general transformation $g = g(\mathbf{q}, \mathbf{p})$, this last example motivates one to examine forms of g involving the kinetic energy T as well as F:

$$g = \frac{1}{\lambda T + \mu F} \tag{2.28}$$

where $\lambda, \mu > 0$ are constants. Again, there exists the explicit relation (cf. [37])

$$t = \frac{1}{(\lambda + 2\mu)h}\left[(\lambda + \mu)\sum_{i=1}^{N} (\mathbf{p}_i')^T \mathbf{q}_i' - s\right] + \text{constant}. \tag{2.29}$$

The equations of motion in physical variables $(\mathbf{q}_{ij}, \mathbf{p}_{ij})$ in terms of parametrized time s may easily be derived from those given in [37]:

$$\begin{aligned} \frac{d\mathbf{q}_{ij}}{ds} &= g\frac{\partial H}{\partial \mathbf{p}_{ij}} + (H - h)\frac{\partial g}{\partial \mathbf{p}_{ij}} \\ &= g[1 - \lambda g(H - h)]\frac{\partial H}{\partial \mathbf{p}_{ij}} \end{aligned} \tag{2.30}$$

$$\begin{aligned} \frac{d\mathbf{p}_{ij}}{ds} &= -g\frac{\partial H}{\partial \mathbf{q}_{ij}} - (H - h)\frac{\partial g}{\partial \mathbf{q}_{ij}} \\ &= -g[1 + \mu g(H - h)]\frac{\partial H}{\partial \mathbf{q}_{ij}}. \end{aligned} \tag{2.31}$$

The corresponding equations in regularized variables $(\mathbf{Q}_{ij}, \mathbf{P}_{ij})$ can be found from Eqs. (2.30)–(2.31) using the KS-transformation (2.1)–(2.4) [20]

$$\frac{d\mathbf{Q}_{ij}}{ds} = \frac{\partial \Gamma^*}{\partial \mathbf{P}_{ij}} = \frac{\partial \Gamma^*}{\partial \mathbf{p}_{ij}}\frac{\partial \mathbf{p}_{ij}}{\partial \mathbf{P}_{ij}} = \frac{1}{4R_{ij}} A(\mathbf{Q}_{ij})\frac{d\mathbf{q}_{ij}}{ds} \tag{2.32}$$

$$\begin{aligned} \frac{d\mathbf{P}_{ij}}{ds} &= -\frac{\partial \Gamma^*}{\partial \mathbf{Q}_{ij}} = -\frac{\partial \Gamma^*}{\partial \mathbf{q}_{ij}}\frac{\partial \mathbf{q}_{ij}}{\partial \mathbf{Q}_{ij}} - \frac{\partial \Gamma^*}{\partial \mathbf{p}_{ij}}\frac{\partial \mathbf{p}_{ij}}{\partial \mathbf{Q}_{ij}} \\ &= A(\mathbf{Q}_{ij})\frac{d\mathbf{p}_{ij}}{ds} - \frac{1}{4R_{ij}} A(\mathbf{P}_{ij})\frac{d\mathbf{q}_{ij}}{ds} + \frac{4T_{ij}}{R_{ij}}[1 - \lambda g(H - h)]\,\mathbf{Q}_{ij} \end{aligned} \tag{2.33}$$

where the last term arises from

$$\frac{1}{2}\mathbf{p}_{ij}\frac{\partial H}{\partial \mathbf{p}_{ij}} \equiv T_{ij}; \qquad \sum_{i<j}\sum T_{ij} = T.$$

The case $\lambda = \mu = 1$ gives rise to the Lagrangian time transformation

$$g = 1/L \tag{2.34}$$

considered by Szebehely and Zare [37], Mikkola [20, 25] (in conjunction with the Heggie regularization scheme), and others. It will be considered in this paper with both Heggie and Aarseth–Zare schemes with regularization, as well as the Aarseth–Zare scheme without regularization (cf. Eqs. (2.30)–(2.31)).

In the vicinity of a collision, the transformation (2.28) has the behaviour $g \sim (t_c - t)^{2/3}$, and hence the singularity now occurs in the equations for $d\mathbf{p}_{ij}/ds$ ($\sim (s_c - s)^{-2}$) or $d\mathbf{P}_{ij}/ds$ ($\sim (s_c - s)^{-1}$), as follows from Eqs. (2.16) and (2.17).

Finally, from the equations of motion (2.10)–(2.11), written in the form

$$\begin{aligned} \frac{d\mathbf{Q}_{ij}}{ds} &= g\frac{\partial H}{\partial \mathbf{P}_{ij}} + (H-h)\frac{\partial g}{\partial \mathbf{P}_{ij}} \\ \frac{d\mathbf{P}_{ij}}{ds} &= -g\frac{\partial H}{\partial \mathbf{Q}_{ij}} - (H-h)\frac{\partial g}{\partial \mathbf{Q}_{ij}} \end{aligned} \tag{2.35}$$

we note the appearance of Poincarré control terms [6] in the second terms of the right-hand sides. Along an exact solution, these terms are zero. If we generalize these control terms to have the form

$$(H-h)\,\mathbf{Y}_{ij}, \qquad -(H-h)\,\mathbf{Z}_{ij}$$

then, in order that departures from the exact integral of motion $H - h = 0$ due to numerical truncation and round-off errors diminish with time, these terms must have the property [6]

$$\begin{aligned} \frac{d}{ds}\left[\frac{1}{2}(H-h)^2\right] &= (H-h)\sum_{i<j}\left(\frac{\partial H}{\partial \mathbf{Q}_{ij}}\frac{d\mathbf{Q}_{ij}}{ds} + \frac{\partial H}{\partial \mathbf{P}_{ij}}\frac{d\mathbf{P}_{ij}}{ds}\right) \\ &= -\frac{(H-h)^2}{g}\sum_{i<j}\left(\mathbf{Z}_{ij}\frac{d\mathbf{Q}_{ij}}{ds} + \mathbf{Y}_{ij}\frac{d\mathbf{P}_{ij}}{ds}\right) \\ &< 0 \end{aligned}$$

or, equivalently,

$$\sum_{i<j}\left(\mathbf{Z}_{ij}\frac{d\mathbf{Q}_{ij}}{ds} + \mathbf{Y}_{ij}\frac{d\mathbf{P}_{ij}}{ds}\right) > 0. \tag{2.36}$$

The control terms in (2.35) have the form

$$\mathbf{Y}_{ij} = \frac{\partial g}{\partial \mathbf{P}_{ij}}; \qquad \mathbf{Z}_{ij} = \frac{\partial g}{\partial \mathbf{Q}_{ij}} \tag{2.37}$$

so in this case we have [37]

$$\frac{d}{ds}\left[\frac{1}{2}(H-h)^2\right] = -(H-h)^2 \frac{1}{g}\frac{dg}{ds}. \tag{2.38}$$

Therefore, stabilization of the integral $H-h=0$ can only occur when g is increasing along the solution path. This condition is satisfied for the Lagrangian time transformation (2.34) only while L is decreasing, following a close encounter. Regardless of the functional form of g, a given method may be stabilized by means of the simple device introduced by Zare and Szebehely [37] of using the control terms (2.37) but reversing the sign on each whenever g was found to be decreasing. It is clear that exactly the same considerations apply to the general equations using the time transformation without regularization, as in Eqs. (2.30) and (2.31).

3. Numerical Tests of Proposed Methods

In order to test the performance of the methods described in Section 2, the standard techniques of (i) time-reversal tests on critical many-body close encounters [5, 10] and (ii) comparison with known analytic solutions [37] were used. A further test for consistency between different methods is to integrate through a resonance scattering event and compare the outcomes, using the same initial conditions for each method. The first two techniques are described below, and results of numerical tests are presented; the third technique is discussed in Section 4.

In order to establish notation, the following conventions are used:

1. Aarseth–Zare type methods (with KS-regularisation) are denoted by "AZ"; Heggie type methods by "H." If regularisation is not used, there is an additional qualifier "C."

2. Methods which use time transformations involving the interparticle separations only are specified by "R"; while "P" denotes the "product" transformation (2.13). The letter "T" denotes the transformation (2.23) which attempts to smooth triple collisions.

3. The letters "L" and "U" specify time transformations involving the Lagrangian and potential energy functions, respectively.

4. The letter "S" specifies that the method has been energy-stabilized using the Zare–Szebehely technique (Section 2).

5. A numerical "n" indicates that the method is specific to a system of n bodies.

TABLE I

Methods for Numerical Integration of the Gravitational N-Body Problem

Method	Equation in text	No. of equations	Method	Equation in text	No. of equations
HR, HRS	(2.21)	$4N(N-1)+1$	AZR, AZRS	(2.22)	$8(N-1)+1$
HL, HLS	(2.34)	$4N(N-1)$	AZL, AZLS	(2.34)	$8(N-1)$
HRP, HRPS	(2.13)	$4N(N-1)+1$	AZRP, AZRPS	(2.13)	$8(N-1)+1$
HRT4	(2.23)	49	AZU	(2.26)	$8(N-1)$
C4*	($g=1$)	24	AZCL*	(2.34)	$8(N-1)$

Note. Methods listed were tested using (i) time reversal of a critical many-body encounter, (ii) comparison with analytic solution, and (iii) integration through a resonance scattering event. Tests included both the 3- and 4-body systems. See text for explanation of the notation. All methods except those marked with an asterisk employ KS-regularization.

Thus, for example, AZLS denotes an Aarseth–Zare-type method (with KS-regularization) using a Lagrangian time transformation and stabilization. The methods that were tested are listed in Table I.

To allow for the possibility of frequent step-size changes during integrations, a Runge–Kutta integrator of eight-order due to Fehlberg [7] was used. This integrator provides an estimate of the absolute truncation error ε, measured as the maximum component of the error vector output after each step. This error was used to define the new time step in terms of the old one according to

$$\Delta s_{\text{new}} = (\eta/\varepsilon)^{1/9} \Delta s_{\text{old}} \tag{3.1}$$

where η is the absolute error tolerance specified as input to the program.

A useful quantity that is easy to compute and allows one to follow some of the qualitative features of the dynamics is the total perimeter of the system, defined as

$$\sigma = \sum_{i<j} \sum R_{ij} \tag{3.2}$$

where the sum extends over all particle pairs. This definition of "perimeter" is different to the one used in [14], but for regularized schemes is more convenient since it avoids the computation of square roots (see Eq. (2.3)).

At this stage, a number of important points should be emphasized. Numerical comparisons between different methods cannot unambiguously establish any method as being superior to another. The performance of a given method depends at least on the following factors:

(a) The type of test applied;

(b) The type of numerical differential equation solver used;

(c) The size of the error tolerances specified, and—perhaps more significantly the manner in which the error at each integration step is both estimated and controlled. Often, as in [14], the error which is controlled is the deviation of total energy, and the step-size is estimated from consideration of the dynamics of the system. Since the integrator used in the present paper provides an estimate of the local truncation error, this was preferred as a means of step-size control (Eq. (3.1.)).

(d) A further complication arises from the nature of the N-body problem itself, which is "unstable" in the sense of exhibiting sensitivity to initial conditions. The consequences of this for numerical integrations are well known [17, 26], and will be discussed later.

3.1. *Time Reversal Tests on Close Many-Body Encounters*

Time-reversal tests were carried out on both 3- and 4-body systems. Although the former have been investigated before [5, 10], these tests included only a subset of the present methods, and a uniform comparison of all these methods is justified.

Triple encounters in a 3-body system were generated from an initial configuration consisting of a distorted equilateral triangle, with particles of unit mass located at rest at the positions $(\pm 1 - \frac{1}{2}\delta x, \ -1/\sqrt{3})$ and $(\delta x, \ 2/\sqrt{3})$. The system was integrated forward in time until a binary was formed with orbital semi-major axis a and eccentricity e, such that the nearest particle to the binary was at a distance $>20a$. At this time $t = T_f$, the velocities of the particles were reversed, and the system integrated forward for a length of time T_f, after which the initial and final configurations were compared. For methods in which t appears as a dependent variable, it was necessary to iterate the solution until $t = T_f$. The magnitude of the residuals between initial and final position is defined as the maximum difference over all coordinates and all particles, and is given in Table III for two initial configurations. The smaller the δx in the initial configuration, the smaller will be the minimum perimeter of the 3-body system and thus the more stringent the test. This minimum perimeter $\sigma(\min)$ and the binary orbital parameters a and e agreed among the different methods to at least 4 significant figures, and are given in Table II.

TABLE II

3-Body Time-Reversal Tests

Configuration	δx	a	e	$\sigma(\min)$	$\sigma(\min)/a$
T1	1.0 (−4)	0.4504 (−3)	0.6180	0.1322 (−2)	2.935
T2	1.0 (−6)	0.8255 (−5)	0.6171	0.2423 (−4)	2.935

Note. Particles of unit mass are started from rest at the vertices of a distorted equilateral triangle, where δx is the distortion (see text). The system evolves through a close triple encounter, as a result of which a binary forms with orbital semi-major axis a and eccentricity e. $\sigma(\min)$ is the smallest perimeter of the system during the close encounter.

TABLE III

Time-Reversal Tests on a Close 3-Body Encounter:
Initial Configurations T1 and T2 Defined in Table II

Method	Configuration T1			Congiguration T2		
	Δx	ΔE	No. of steps	Δx	ΔE	No. of steps
HRS	0.11 (−6)	0.12 (−4)	215	0.13 (−5)	0.13 (−2)	233
HR	0.33 (−8)	0.31 (−5)	125	0.88 (−6)	0.22 (−2)	134
AZRS	0.33 (−7)	0.68 (−7)	230	0.44 (−6)	0.82 (−5)	249
AZR	0.45 (−8)	0.57 (−6)	144	0.38 (−7)	0.70 (−4)	155
HRPS	0.39 (−8)	0.69 (−6)	267	0.15 (−6)	0.99 (−3)	299
HRP	0.53 (−6)	0.27 (0)	214	0.42 (−3)	0.45 (+5)	247
AZRPS	0.14 (−7)	0.29 (−7)	262	0.18 (−6)	0.48 (−5)	287
AZRP	0.17 (−6)	0.43 (−4)	183	0.12 (−3)	0.13 (0)	202
HLS	0.49 (−8)	0.18 (−6)	218	0.42 (−6)	0.56 (−3)	235
HL	0.27 (−8)	0.70 (−6)	151	0.71 (−6)	0.17 (−2)	156
AZLS	0.25 (−8)	0.98 (−8)	229	0.35 (−7)	0.25 (−5)	245
AZL	0.11 (−8)	0.23 (−6)	161	0.15 (−7)	0.13 (−4)	168
AZCL	0.11 (−9)	0.11 (−8)	521	0.19 (−9)	0.70 (−8)	707

Note. The integrations are reversed at time $t = T_f$ when the nearest particle to the binary formed by the close encounter is at a distance $>20a$, where a is the orbital semi-major axis of the binary. The maximum of the residuals in final position (among the 3 components of all particles) is Δx, and the size of maximum deviation of total energy, during integrations, from constant (initial) value is ΔE. The error tolerance for each method is 10^{-12}. The number of steps required to reach $t = T_f$ is given. All integrations were carried out on a FPS-164, which has 15 decimal place accurate floating point arithmetic.

From Table III, it can be seen that for each method, introducing energy-stabilization does indeed reduce the maximum deviation of the total energy from its constant (initial) value. However, in the case of the "optimal" methods HR and AZR, stabilization actually leads to larger residuals in position. Furthermore, stabilized methods seem to require more steps (at slightly extra cost per step) than their non-stabilized counterparts. The non-regularized method AZCL appears to require more than twice as many steps as the least efficient of the regularized methods, with this ratio being larger for the more critical encounter T2. For the same absolute error tolerances as the regularized methods, AZCL also gives the smallest residuals in position and total energy. Finally, note that the perimeter of the 3-body system is close to $3a$ for both sets of initial conditions. This well-known result was also found by numerical tests in [5], and is a consequence of Sundman's inequality [33].

The initial conditions for time-reversal tests on 4-body encounters were chosen to be the vertices of a distorted regular tetrahedron, with particles of unit mass located at rest at the positions $(\pm\frac{1}{2}, -1/2\sqrt{3} \pm \delta y, -1/2\sqrt{6} - \delta z)$, $(0, 1/\sqrt{3}, -1/2\sqrt{6} - \delta z)$, and $(0, 0, \sqrt{3}/2\sqrt{2} + 3\delta z)$. As in the 3-body case, a close binary forms during the critical encounter, and the forward integrations were stopped

TABLE IV

4-Body Time-Reversal Tests

Configuration	δy	δz	a	e	σ(min)	$\sigma^{(3)}$(min)	$\sigma^{(3)}$(min)/a
QT1	1.(−3)	0.2	0.3290(−2)	0.6308		0.973(−2)	2.96
QT2	1.(−4)	0.2	0.4465(−3)	0.6180		0.131(−2)	2.93
QT3	1.(−6)	0.2	0.8185(−5)	0.6159		0.241(−4)	2.94
Q1	1.(−3)	5.(−3)	0.2674(−2)	0.5808	0.182(0)	0.775(−2)	2.90
Q2	1.(−3)	1.(−3)	0.2703(−2)	0.3762	0.479(−1)	0.742(−2)	2.75
Q3	1.(−4)	1.(−4)	0.3625(−3)	0.3487	0.644(−2)	0.962(−3)	2.65
Q4	1.(−5)	1.(−5)	0.4864(−4)	0.3380	0.869(−3)	0.127(−3)	2.61
Q5	1.(−7)	1.(−7)	0.8812(−6)	0.3294	0.159(−4)	0.288(−5)	2.59

Note. The particles, of unit mass, are started from rest at the vertices of a distorted regular tetrahedron, where δy, δz are the distortions (see text). The system evolves through a close triple or quadruple encounter (for initial configurations "QTn" and "Qn," respectively). A binary forms with orbital semi-major axis a and eccentricity e. σ(min) is the minimum perimeter of the total system, $\sigma^{(3)}$(min) that of the smallest 3-body subsystem, during the close encounter.

when the nearest particle to the binary was at a distance $>100a$. By choosing the initial conditions so that $|\delta y|$ and $|\delta z|$ are of the same order of magnitude, a critical 4-body close encounter can be simulated; while if $|\delta z| \gg |\delta y|$, then a critical 3-body encounter occurs. In the former case, the minimum total perimeter σ(min), as well as the minimum perimeter $\sigma^{(3)}$(min) formed from the closest 3-particle subsystem, is of interest; in the latter case, only $\sigma^{(3)}$(min) has significance.

Several configurations, defined by different sets of $(\delta y, \delta z)$ values, were integrated, and the binary and minimum perimeters characteristic of each method are given in Table IV. Again, agreement in these values to at least 4 significant digits was found for all methods. Results of the integrations for each of the methods are given in Tables V and VI only for the 3 most critical cases. In some instances, a method would "fail," in the sense of requiring more than 5 minutes of FPS-164 CPU time and of showing large residuals of total energy in the course of integration. For example, for the initial conditions of Table V, leading to a close triple encounter in the 4-body system, the method HRT4 (Eq. (2.23)), which is designed to handle 3-body close encounters in an "optimal" way, gave smaller residuals than either HR and HRS (Eq. (2.24)) which are optimal for close 4-body encounters. Conversely, HRT4 failed, whereas HR and HRS succeeded, in the two most critical 4-body encounters given in Table VI. This example alone demonstrates the effectiveness of employing "optimal" time transformations, in terms of requiring fewer steps to achieve a given accuracy. It also demonstrates a drawback of the class of time transformations based only on the R_{ij}'s and represented by Eqs. (2.13), (2.23), and (2.24): whether or not the transformation is optimal depends on the number of bodies involved in the close encounter. Furthermore, methods which are not optimal for a given type of close encounter (including AZRP and HRP, which

TABLE V

Time-Reversal Tests on a Close Triple Encounter in a 4-Body System: Initial Configuration QT3 Defined in Table IV

Method	Δx	ΔE	No. of steps
HRT4	0.87 (−7)		335
HRS	0.65 (−5)	0.22 (0)	594
HR	0.43 (0)	0.21 (+5)	396
AZRS	0.52 (−5)	0.14 (−3)	558
AZR	0.64 (−4)	0.12 (0)	339
HRPS	0.81 (−5)	0.16 (0)	599
HRP	*	*	*
AZRPS	0.49 (−5)	0.60 (−4)	570
AZRP	0.37 (−3)	0.13 (+1)	354
HLS	0.13 (−4)	0.17 (0)	597
HL	0.60 (−3)	0.13 (+1)	420
AZLS	0.43 (−6)	0.60 (−5)	595
AZL	0.21 (−5)	0.27 (−3)	414
AZU	0.44 (−3)		324
AZCL	0.10 (−8)	0.63 (−7)	1750
C	0.13 (−6)		2069

Note. The integrations are reversed at time $t = T_f$, when the nearest particle to the binary formed in the close encounter is at a distance $> 100a$, where a is the orbital semi-major axis of the binary. The maximum of the residuals in the final position (among the 3 components of all particles) is denoted by Δx, and the size of maximum deviation of the total energy from constant (initial) value is denoted by ΔE. The error tolerance for each method is 10^{-11}. The number of steps required to reach T_f is given. If a method failed to converge after 5 minutes of processing time, this is denoted by an asterisk. All integrations were carried out on a FPS-164, which has 15 decimal places of accuracy of floating point arithmetic.

are optimal (regular) only for 2-body encounters) show a definite improvement in accuracy of final position when energy-stabilization is introduced. In many cases, a stabilized version would converge, whereas its non-stabilized counterpart would fail. The effectiveness of stabilization in optimal methods is not as clear, as has been found by others (for example, [4] for the 3-body case).

Integration of the classical equations (method C4) appears to offer no advantage in accuracy or efficiency, even compared to AZCL.

It is evident from an examination of Tables V and VI that methods based on the Lagrangian time transformation, Eq. (2.34), possess the best advantages of accuracy and efficiency. As noted earlier, the behaviour of these methods near multiple collisions is independent of the number of bodies involved in the collision. When comparing the different methods based on the Lagrangian time transformation, it is interesting to note that the Aarseth–Zare-type schemes appear to exhibit smaller residuals than those based on the Heggie-type scheme. This is true of both the 3- and 4-body cases tested. The two schemes require comparable numbers of steps for a given initial configuration, but the Aarseth–Zare schemes have fewer equations

than the Heggie schemes, and are therefore less costly to use. When considering the non-regularized method AZCL, twice as many steps were required than the KS-regularized counterpart AZL, though for the same absolute error tolerance greater accuracy was achieved. However, it was found that, by increasing the error tolerance until the residuals in final position given by AZCL were the same as those produced by AZL for a smaller error tolerance, the two methods required about the same numbers of steps.

The advantages of introducing energy-stabilization into methods employing the Lagrangian time transformation are not as clear as they were for the "non-optimal" methods using time transformations based on the R_{ij}'s only. However, some improvement was found in all cases considered, in terms of the residuals in both total energy and final position.

Finally, as in the 3-body case, there seems to exist a close correlation between the orbital semi-major axis of the binary formed in a close encounter and the minimum perimeter $\sigma^{(3)}(\min)$ defined above: the ratio $\sigma^{(3)}(\min)/a$ is slightly less than 3 for all initial configurations considered (whether a 3- or a 4-body close encounter was being simulated). This ratio, as well as the values of a and e, decreases slowly as the size of the perturbations δy, δz in the initial configuration decreases. Even in close 4-body encounters (Table VI), we have $\sigma(\min) \gg \sigma^{(3)}(\min)$: this seems to suggest that the binary is formed through 3-body, rather than 4-body, interactions.

TABLE VI

Time-Reversal Tests on a Close 4-Body Encounter:
Initial Configurations Q4 and Q5 Defined in Table IV

Method	Configuration Q4			Configuration Q5		
	Δx	ΔE	No. of steps	Δx	ΔE	No. of steps
HRT4	*	*	*	*	*	*
HRS	0.39 (−5)	0.27 (−1)	1054	0.46 (−5)	0.56 (−1)	1816
HR	0.42 (−5)	0.23 (−2)	671	0.16 (−3)	0.94 (−1)	1155
AZRS	0.77 (−5)	0.54 (−5)	995	0.26 (−6)	0.13 (−5)	1755
AZR	0.11 (−5)	0.15 (−3)	641	0.67 (−7)	0.16 (−3)	1110
HRPS	0.90 (−5)	0.23 (−1)	1122	0.78 (−5)	0.11 (0)	1991
HRP	*	*	*	*	*	*
AZRPS	0.73 (−5)	0.65 (−5)	3866	*	*	*
AZRP	0.98 (−2)	0.32 (+3)	3593	*	*	*
HLS	0.28 (−6)		1150	0.51 (−6)	0.58 (−1)	1957
HL	0.36 (−5)	0.62 (−3)	923	0.36 (−5)	0.31 (−1)	1509
AZLS	0.17 (−6)	0.95 (−5)	1151	0.24 (−7)	0.11 (−5)	1929
AZL	0.19 (−5)	0.99 (−4)	875	0.22 (−6)	0.50 (−4)	1432
AZU	0.12 (0)		630	*	*	*
AZCL	0.55 (−5)	0.44 (−3)	1240	0.10 (−7)	0.63 (−6)	6386
C	0.13 (−6)		2995	0.15 (−7)		6630

Note. See Table V for explanation of notation. Error tolerance is 10^{-11} for Q4 and 10^{-13} for Q5.

3.2. *Comparison with Analytic Solutions*

For the 3- and 4-body problems, a variety of configurations exist in which the symmetry is preserved with time. For example, in the 3-body case, there is the equilateral triangle solution of Lagrange, in which each particle executes a Keplerian orbit of semi-major axis a and eccentricity e about the common centre-of-mass, when viewed in a uniformly rotating reference frame with rotation period $P = 2\pi/\Omega$ [8, 37]. The initial conditions were chosen with the particles at the apapses of their orbits, with $a = 1/\sqrt{3}$, which is equivalent to an equilateral triangle with sides of length $(1 + e)$. The particle masses and gravitational constant were chosen to be 1, so the value of Ω is then $\sqrt{3}$.

Similarly, the planar 4-body problem with equal masses possesses an invariant square-symmetric configuration, in which individual particles move in Keplerian orbits about the common centre-of-mass. The initial conditions were again chosen with the particles located at the apapses of their orbits, forming a square configuration with sides of length $\sqrt{2}(1 + e)$. The orbital period (when all masses are 1) is then given by $P = 2\pi/\Omega$, where $\Omega^2 = (2\sqrt{2} + 1)/4$, and $a = 1$.

In both the 3- and 4-body problems, the integrations were carried out for two orbital periods P, with eccentricities $e = 0$ and $e = 0.95$, and the final positions and velocities compared with their initial values. As was the case with the time-reversal tests, for methods in which t appeared as dependent variable, it was necessary to approach the final value $t = 2P$ by iteration. The results are shown in Tables VII and VIII for 8 different methods: stabilization was included only for the "product transformation" methods (cf. Eq. (2.13)) which showed marked improvement over their non-stabilized counterparts in the time-reversal tests of Section 3.1 above.

TABLE VII

Comparison with Analytic Solutions: Residuals in Position (Δx) and Velocity (Δv) after Two Orbital Periods for the Lagrange Equilateral Triangle Solution of the 3-Body Problem

Method	$e = 0$			$e = 0.95$		
	No. of steps	Δx	Δv	No. of steps	Δx	Δv
HR	44	0.35 (−10)	0.56 (−10)	80	0.35 (−8)	0.57 (−8)
AZR	49	0.21 (−10)	0.31 (−10)	84	0.48 (−8)	0.79 (−8)
HRPS	84	0.11 (−9)	0.21 (−9)	185	0.19 (−8)	0.14 (−8)
AZRPS	48	0.24 (−9)	0.40 (−9)	92	0.11 (−7)	0.30 (−7)
HL	53	0.18 (−10)	0.29 (−10)	85	0.11 (−8)	0.97 (−9)
AZL	60	0.11 (−10)	0.19 (−10)	93	0.25 (−8)	0.33 (−8)
AZU	52	0.16 (−10)	0.28 (−10)	87	0.28 (−8)	0.20 (−8)
AZCL	83	0.46 (−10)	0.11 (−9)	161	0.20 (−8)	0.14 (−8)

Note. All masses are unity; period $P = 2\pi/\sqrt{3}$; $a = 1/\sqrt{3}$. Absolute error tolerance in the integrations is 10^{-11}. Only the "product transformations" (cf. Eq. (2.13)) were stabilized, as the time-reversal tests (Tables V and VI) indicated that the methods were significantly improved compared to their non-

TABLE VIII

Comparison with Analytic Solutions: Residuals in Position (Δx) and velocity (Δv) after Two Orbital Periods for the Planar Square-Symmetric Solution of the 4-Body Problem with Equal (Unit) Masses

Method	$e=0$			$e=0.95$		
	No. of steps	Δx	Δv	No. of steps	Δx	Δv
HR	47	0.52 (−10)	0.45 (−10)	83	0.21 (−7)	0.99 (−8)
AZR	53	0.19 (−10)	0.16 (−10)	91	0.27 (−7)	0.13 (−7)
HRPS	111	0.24 (−9)	0.16 (−9)	289	0.16 (−7)	0.70 (−8)
AZRPS	63	0.11 (−9)	0.10 (−9)	140	0.43 (−7)	0.30 (−7)
HL	53	0.28 (−10)	0.24 (−10)	85	0.53 (−8)	0.27 (−8)
AZL	62	0.16 (−10)	0.14 (−10)	98	0.27 (−7)	0.12 (−7)
AZU	57	0.20 (−10)	0.18 (−10)	96	0.31 (−7)	0.14 (−7)
AZCL	86	0.52 (−10)	0.45 (−10)	145	0.22 (−7)	0.83 (−8)

Note. Period $P=2\pi/\Omega$, where $\Omega^2=(2\sqrt{2}+1)/4$, $a=1$. Absolute error tolerance in the integrations is 10^{-11}. Only the "product transformations" (cf. Eq. (2.13)) were stabilized, as the time-reversal tests (Tables V and VI) indicated that the methods were significantly improved compared to their non-stabilized counterparts.

From these tables, it appears that Lagrangian time-smoothing applied to both Heggie and Aarseth–Zare methods with regularisation (HL, AZL) gives the best results, with the former showing appreciably higher accuracy than the latter for the $e=0.95$ cases. The methods employing the "product transformation" (2.13) displayed both the least accuracy and the highest number of integration steps. The advantage of regularized over non-regularized methods is evident even for the mildly critical encounters occuring in this test, when one compares HL and AZL for the $e=0.95$ case with AZCL.

4. 3- and 4-Body Scattering Experiments

In this section, a computer program will be described for studying binary-single star or binary-binary scattering. Similar programs have recently been developed by Hut and Bahcall [14, 15] in their study of 3-body scattering and by Mikkola [21–24, 25] in a study of 4-body scattering, though in each case different criteria were used to decide when to terminate integrations due to one or other type of scattering outcome occurring. As far as the present paper is concerned, such a program is useful in providing yet another test of the various methods proposed in Section 2 above for integrating through close encounters involving 2 or more bodies.

Experiments on scattering involving hard binaries provide a useful test of any scheme for numerically integrating an orbit, because of the frequent occurrence of resonances. They also highlight fundamental difficulties associated with long-term integrations of N-body problems [17, 26]. Therefore, experiments were carried out

with hardness parameter x having the values 10^2 and 10^4, where x is defined as the ratio of total binding energy of the binary or binaries to the kinetic energy of relative motion of the binary + single star (3-body case) or binary + binary (4-body case) before scattering. Also, the masses of all stars were chosen to be unity, and the initial binary orbit(s) to have semi-major axis of unity and eccentricity of zero. The gravitational constant was chosen to be unity. The impact parameter for the scattering (measured with respect to the centre-of-mass of the binary or binaries) was set at $\rho = 0.01$. In each of the 3- and 4-body cases, the same initial conditions were used for all methods tested, though in a statistical study of many scattering experiments different initial conditions could be generated by the program by sampling the incoming scattering angles and orientation and phases of the binary orbit(s) from the appropriate distributions [14].

The initial conditions for a 3-body scattering experiment were defined in the same way as in [14, Fig. 1]. Initial conditions for binary-binary scattering were defined in an analogous way, except now four more angles need to be specified and randomly chosen from the appropriate distributions. These are the inclination; longitude of ascending node; argument of periastron of the second binary referred to axes through the centre-of-mass of the first binary, with x-axis along the direction of periastron and the xy-plane coinciding with the orbital plane; and the orbital phase of the second binary at periapsis of the unperturbed hyperbolic relative orbit of the two binaries. This approach is a convenient one for generating a reproducible sequence of initial conditions, when running large numbers of experiments for obtaining scattering cross sections in 3- and 4-body system.

For a particular set of initial conditions, the 3- or 4-body system was integrated until a definite outcome was obtained. For the 3-body case, the number of possible outcomes is small: ionization, fly-by, exchange of the incoming particle with one of the binary components, or a hierarchical triplet. In the first case, all 3 particles eventually escape to infinity; in the second the original binary remains intact; in the third, a binary is also left behind but with different components. In binary-binary scattering, several more possibilities exist: ionization, two binaries remaining intact (with or without their original components), or only one of the binaries remaining intact. Also, hierarchical triplets or quadruplets may form, which are in principle unstable, but may survive an indefinitely long time before breaking up into one of the stable configurations mentioned above. Therefore, an upper limit must be set to the number of oscillations of the perimeter σ during a given orbit integration, as was done in [14]. Alternatively, an upper limit to the total physical time t, in terms of a fixed number of orbital periods of the initial binary, could be set.

The criteria chosen for terminating hierarchical configuration integrations were different for 3- and 4-body systems. For a 3-body system, Zare's criterion [34, 36] was used. A critical value $(c^2H)_{cr}$ (c = total angular momentum, H = total energy) was computed from the collinear central configuration and compared with the actual value of c^2H: if this was greater than the critical value, integrations were terminated with the outcome of a stable hierarchy. This criterion is equivalent to a lower bound on the ratio of the semi-major axes of the outer to the inner binary,

though this ratio depends senstively on the orbital eccentricities when they are close to unity (as is often the case in scattering). Note that Zare's criterion is strictly applicable only if the two binary orbits are coplanar. For the 4-body hierarchical system, consisting of either 3 hierarchical binaries or two binaries in wide (bound) orbit about each other, a simpler criterion was used: if the perturbation acceleration of one orbit on another was less than 10^{-4} of the two-body acceleration, the system was regarded as hierarchically stable and the integrations stopped. This is also the criterion used by Mikkola [21]. However, several hundred preliminary runs at various impact parameters indicate that, for hard binaries at least, such 4-body hierarchical configurations are much less likely to occur than 3-body ones.

The number of successive maxima and minima of σ before an outcome is established indicates the degree of complexity of the resonance scattering. Often, this number is several hundreds or thousands, requiring of the order of 10^4 integration steps, depending on the method used.

A well-established feature of binary-binary scattering [29] is that in most cases the system would go unstable by ejecting one particle, rather than ejecting a bound binary system. Thus, a strongly interacting 3-body subsystem would be left behind, which in turn would eventually go unstable. Therefore, the subroutines for a 3-body system were incorporated in the 4-body program. The criteria used for escape were (i) the distance between the outermost particle and the centre-of-mass of the 3-body subsystem was increasing and (ii) the energy of the Keplerian orbit of this particle (call it "4") about the centre-of-mass of the other three exceeds a positive threshold defined as the tidal perturbation energy $|E_{\text{tid}}|$ of the inner 3 particles on the outer particle:

$$E_{\text{tid}} = Gm_4\left(\frac{m_1}{R_{14}} + \frac{m_2}{R_{24}} + \frac{m_3}{R_{34}} - \frac{(m_1 + m_2 + m_3)}{\bar{R}}\right) \tag{4.1}$$

where $\bar{R}$ denotes the distance to the centre-of-mass of particles 1, 2, 3. Once both these criteria were found to be satisfied, the integrations were continued for another 20 steps and the criteria re-checked. If still satisfied, the particle was deemed to have escaped. Similar criteria were applied to decide the escape of stars from a 3-body system, and of binaries from a 4-body system. It should be noted that, in the 3-body case, several alternative, sufficient conditions for escape exist: for example, see [31]. These could, in principle, be adapted to the 4-body case to obtain a less rigorous but still practical criterion if a hard binary is present and may be treated as a single particle.

In a 3-body system, in which a close and wide binary form, in many cases the eccentricity of the wide orbit is close to unity, so that at periapsis the particle in wide orbit undergoes a strong interaction with the close pair. However, since most of its time is spent at large distances from the close pair, a 2-body approximation is justified. Therefore, when the separation exceeds 60 times the orbital semi-major axis of the close pair, and this separation is increasing, the 2-body approximation is invoked to compute the orbital phase of the close binary when the outer particle

returns to the same distance after having passed through the apapsis of its orbit. No perturbation treatment is used, as is done in Mikkola's code [21].

In the scattering experiments the incoming particle in binary-single star scattering is labelled "3", and the components of the initial binaries in binary-binary scattering are labelled (1, 2) and (3, 4). The asymptotic relative velocity before scattering v_∞ is conveniently measured in terms of the critical velocity v_c for which the total energy of the system is zero. For the binary-single star case,

$$v_c^2 = \frac{m_1 m_2 (m_1 + m_2 + m_3)}{m_3 (m_1 + m_2)\, a} \tag{4.2}$$

and for the binary-binary case

$$v_c^2 = \frac{(m_1 + m_2 + m_3 + m_4)}{(m_1 + m_2)(m_3 + m_4)} \left\{ \frac{m_1 m_2}{a_1} + \frac{m_3 m_4}{a_2} \right\} \tag{4.3}$$

where a, a_1, and a_2 are the orbital semi-major axes. For both 3- and 4-body systems, the hardness parameter x, defined in Section 3, is related to v_∞ and v_c by

$$x = (v_\infty / v_c)^{-2}. \tag{4.4}$$

The results of applying several methods to a binary-single star scattering experiment with initial binary hardness $x = 10^4$ and fixed initial conditions are given in Table IX. This scattering experiment is not of long duration ($\sim$9 orbital periods of the initial binary) and not a particularly severe test of the methods. The identity of the escaping particle agrees among all the methods, and the orbital charac-

TABLE IX

Scattering of a Binary and a Single Star, with Impact Parameter $\rho = 0.01$, Binary Hardness Parameter $x = 10^4$

Method	n	No. of oscillations	No. of steps	ΔE	Final binary	
					a	e
HR	1	7	280	0.96 (−8)	0.543	0.976
AZR	1	7	280	0.46 (−9)	0.543	0.976
HL	1	21	300	0.17 (−8)	0.543	0.977
AZL	1	17	280	0.14 (−9)	0.543	0.977
AZU	1	5	140	0.18 (−9)	0.543	0.975
AZCL	1	5	320	0.38 (−8)	0.543	0.970

Note. Initial binary has $a = 1$, $e = 0$; all masses are unity. The initial separation of the binary from the incoming single star is $20a$. As a result of the scattering, particle "n" escapes, leaving behind a binary. If $n = 3$, the original binary remains intact; if $n = 1$ or 2, exchange has taken place. Number of oscillations is the number of oscillations of the perimeter of the 3-body system; ΔE is the maximum deviation of total energy from constant (initial) value during the integrations.

TABLE X

Scattering of a Binary and a Binary, with Impact Parameter $\rho = 0.01$, Binary Hardness Parameter $x = 10^2$

Method	n_2	n	No. of oscillations		No. of steps		ΔE		Final Binary	
			3	4	3	4	3	4	a	e
HR	1	2	100	1	1040	100	0.13 (−2)	0.95 (−10)	0.281	0.628
AZR	0	3	57	1	700	160	0.12 (−8)	0.28 (−9)	0.260	0.644
HRPS	0	2	37	1	860	160	0.46 (−8)	0.12 (−8)	0.106	0.750
AZRPS	0	3	81	1	1300	180	0.68 (−9)	0.12 (−8)	0.214	0.405
HL	2	2	45	3	520	140	0.12 (−3)	0.36 (−8)	0.257	0.969
AZL	1	1	119	3	1380	200	0.13 (−4)	0.47 (−9)	0.265	0.605
AZU	2	1	98	3	1180	200	0.27 (−3)	0.49 (−9)	0.263	0.695
AZCL	3	1	352	1	10460	180	0.43 (−3)	0.23 (−8)	0.251	0.935

Note. Initial binaries have $a = 1$, $e = 0$; all masses are unity. The initial separation of the two binaries from each other is $10a$. As a result of the scattering, particle "4" escapes, leaving behind a 3-body system which eventually decays into a binary and escaping particle "n"; if $n = 3$, one of the original binaries remains intact; if $n = 1$ or 2, exchange has taken place. ΔE is the maximum deviation of total energy from constant (initial) value during the 4-body integrations. n_2 is the number of times the 2-body approximation was called during the 3-body integrations: the relatively large deviations in the total energy of the 3-body system arise from this approximation, which was invoked whenever the distance of the particle in wide orbit was greater than 60 times the separation of the inner pair.

teristics of the final binary are approximately the same. However, the number of oscillations of the perimeter differ widely.

For the binary-binary scattering experiment (Table X), in which $x = 10^2$, the identity of the first escaper is the same in each case, though the number of oscillations of the 4-body perimeter differ. However, the identity of the second escaper does *not* agree among the different methods, and there is not as close agreement regarding the orbital characteristics of the final binary as in the case of binary-single star scattering. This is in part due to phase errors introduced by invoking the 2-body approximation; however, as Table X shows, the 2-body approximation is called different numbers of times for different methods. Even for those methods which do not invoke the approximation, different second escapers are produced. Furthermore, the durations of physical time of scattering show a wide variation: in general, methods which require more oscillations in σ also produced a larger value of the final t.

Runs with several initial conditions in both 3- and 4-body scattering runs clearly show that, whenever strong resonances occur, in which σ undergoes thousands of oscillations, the outcomes can vary with method and with the error tolerance specified for a given method—even when the 2-body approximation is not introduced. On the other hand, if only a few oscillations occur, and the scattering is of short duration, the outcomes agree. This highlights the fundamental difficulty

associated with numerical integrations of N-body gravitational systems: small perturbations—whether due to different error propagation in different integration schemes, or to different tolerances being specified for a given scheme—can lead to widely separated orbits. The divergence is even greater for binary-binary scattering than for binary-single star scattering. This is due partly to the artifact of isolating the 3-body subsystem from the escaping star. This in general will occur at different parts of the orbit for different integration schemes, because the test for isolating the 3-body subsystem is applied only after every 20 steps and step-sizes will differ from one method to another. Hence, the perturbations which are caused by the neglect of the potential field of the escaping star, though small, are not zero, and sensitivity to these small perturbations will cause the orbits to diverge by amounts which increase as the duration of the scattering increases.

5. Discussion

The scattering experiments discussed in Section 4 serve to illustrate the inherent instability of the gravitational N-body problem, even when N is as small as 3 or 4. The divergence in phase space of neighboring orbits over long periods of time can lead to widely varying outcomes as to the identity and kinetic energy of the escaping star, as has been shown by the numerical experiments of Lecar [17] and Miller [26]. The best that can be hoped is for those N-body orbits which undergo large numbers of oscillations in σ to fill the asymptotic regions of phase space (occupied by the different categories of scattering outcomes) with a good approximation to the correct distribution, when a large number of experiments are performed.

Comparison of the methods proposed in this paper with analytic solutions and by means of time-reversal tests point to the superiority of methods based on the Lagrangian time transformation, which combines the advantages of accuracy, efficiency, and independence of performance on the number of bodies involved in a particular many-body close encounter. There appears to be no advantage in accuracy or fewer numbers of steps required for the Heggie scheme, which was used by Mikkola [20, 21], compared with the Aarseth–Zare scheme. In fact, the fewer numbers of equations associated with the latter result in their being less expensive to use than the Heggie-type schemes. Of course, only one criterion was tested for choosing the reference body in the Aarseth-Zare schemes: others should be tried, particularly when the particle masses are different.

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