1
The N-body problem

1.1 Introduction

The main purpose of this book is to provide algorithms for direct N-body simulations, based on personal experience over many years. A brief description of the early history is included for general interest. We concentrate on developments relating to collisional direct integration methods but exclude three- and four-body scattering, which will be discussed in a separate chapter. In the subsequent section, we introduce some basic concepts which help to understand the behaviour of self-gravitating systems. The topics covered include two-body relaxation, violent relaxation, equipartition of kinetic energy and escape. Although the emphasis is on collisional dynamics, some of the theory applies in the large-N limit that is now being approached with modern hardware and improved numerical techniques. After these theoretical considerations, we turn to the problem at hand and introduce the general principles of direct integration as a beginner's exercise and also describe the first N-body method.

1.2 Historical developments

Numerical investigations of the classical N-body problem in the modern spirit can be said to have started with the pioneering effort of von Hoerner [1960]. Computational facilities at that time were quite primitive and it needed an act of faith to undertake such an uncertain enterprise.* Looking

back at these early results through eyes of experience, one can see that the characteristic features of binary formation and escape are already present for particle numbers as small as $N = 16$, later increased to 25 [von Hoerner, 1963]. In the beginning, integration methods were to a large extent experimental and therefore based on trial and error. This had the beneficial effect of giving rise to a variety of methods, since every worker felt obliged to try something new. However, by Darwinian evolution it soon became clear that force polynomials and individual time-steps† were important ingredients, at least in the quest for larger N [Aarseth, 1963a,b].

The basic idea of a force fitting function through the past points is to enable a high-order integration scheme, with the corresponding intervals satisfying specified convergence criteria. Consistent solutions are then ensured by coordinate predictions before the force summation on each particle is carried out. At the same time, the lack of a suitable method for dealing with persistent binaries inspired the introduction of a softened interaction potential $\Phi = -Gm/(r^2 + \epsilon^2)^{1/2}$, for the separation r with ϵ the softening parameter, which reduces the effect of close encounters. This potential gives rise to a simple expression for the force between two particles. Hence a large value of the softening scale length ϵ describes the dynamics of a so-called 'collisionless system', whereas smaller values may be used to exclude the formation of significant binaries. Although the application was to galaxy clusters, some general results on mass segregation were obtained for $N = 100$ and a mass spectrum [Aarseth, 1963a,b].

Later the integration method was improved to third order [Aarseth, 1966a] and eventually became a fourth-order predictor–corrector scheme [Aarseth, 1968], which survived for some considerable time and was widely used. The subsequent study of star clusters by Wielen [1967] was actually based on a fifth-order polynomial with special error control [Wielen, 1974]. This work compared the *extrapolated* half-life of simulated star clusters with observations and concluded that median life-times of about 2×10^8 yr could be accounted for. The nature of the numerical errors is of prime concern in such work and will be considered in a later chapter. In this context we mention that exponential error growth was demonstrated by Miller [1964] in an important paper where the short time-scale was emphasized. This fundamental feature was highlighted in a code comparison study for a collapsing 25-body system [Lecar, 1968]. In fact, these results led many people to question the validity of N-body simulations and this took many years to dispel.

At that time, the lack of computational facilities dictated a strategy of performing a few calculations at the largest possible value of N or

undertaking a systematic study of smaller systems. The latter choice was made by van Albada [1968] and yielded considerable insight into fundamental processes involving binary formation and exchange, as well as the energy of escaping particles. Thus it was demonstrated that a dominant binary containing the heaviest components in systems with up to 24 members sometimes acquires more than 100% of the total initial energy. Some interesting properties of long-lived triples were also presented for the first time, including evidence for the so-called 'Kozai cycle' of induced inner eccentricity (to be discussed later). Small systems are notoriously difficult to integrate but here a special fourth-order predictor–corrector method proved highly accurate, at the expense of *two* force evaluations per step in order to ensure convergence. The same time-step was used for all the particles; however, this becomes expensive above $N \simeq 10$ and the scheme of individual time-steps was never implemented.

By concentrating on just one system and using a dedicated computer, it proved possible to reach $N = 250$ [Aarseth, 1968]. Because of a favourable mass spectrum with two dominant (i.e. factor of 5 in mass) bodies, the final binary acquired some 150% of the *initial* total energy. The softening was still a factor of 10 below the small final semi-major axis, thereby justifying this device which does place a lower limit on binary separation.

The early trend towards greater realism led to the study of two new effects. Since open star clusters move in nearly circular Galactic orbits, the external tidal field can be added to the equations of motion using linearized terms. The first such pure N-body implementation was presented by Hayli [1967, 1969, 1970, 1972]. This work showed the characteristic behaviour of low-energy escaping stars passing near the Lagrange points L_1 and L_2. Again an original method was used called the 'category scheme' [cf. Hayli, 1967, 1969, 1974]. It was never fully developed but has some similarities to the popular Hermite method (to be discussed later).

A second effect relating to open clusters is the perturbation by interstellar clouds. The first attempt for $N = 25$ [Bouvier & Janin, 1970] experienced some technical problems in the boundary treatment, which goes to show that even intuitive selection procedures can be misleading. Moreover, distant particles exaggerated the predicted disruption time based on the change in total energy.[‡] In this case the integration method was again of fourth order with two force evaluations per step.

Among other integration schemes that have served a useful purpose we mention explicit Taylor series based on higher force derivatives. In the context of the N-body problem this idea was implemented by successive differentiations of the Newtonian acceleration [Gonzalez & Lecar, 1968; Lecar, Loeser & Cherniack, 1974]. Although quite accurate, a high-order

[‡] This problem was studied more extensively by Terlevich [1983, 1987].

expansion is too expensive to be practical for $N \geq 10$. On the positive side, the initialization of higher derivatives for standard force polynomials employs the explicit derivative approach to good effect.

In the late 1960s, several efforts were made to take advantage of the two-body regularization formulated by Kustaanheimo & Stiefel [1965; hereafter KS]. It became clear that special treatments of energetic binaries are desirable in order to study the long-term evolution of point-mass systems. One brave attempt to avoid the apparent complications of the KS method for N-body applications was based on the variation of parameters method [Aarseth, 1970]. The dominant central binary that usually emerges was represented by the osculating (or instantaneous) two-body elements. Apart from some problems due to secular perturbations, this method worked quite well.[§] It also had the advantage of permitting unperturbed solutions which speed up the calculation. On the debit side, the method must be replaced by direct integration for significant perturbations. Still, much useful experience of algorithmic decision-making was gained by this application of celestial mechanics.

The impetus for introducing KS regularization was inspired by the beautiful three-body solution illustrated graphically by Szebehely & Peters [1967]. However, the Hamiltonian development of Peters [1968a,b] for the three-body problem bypasses the problem of evaluating the changing energy of the dominant two-body motion by an explicit calculation of the $N(N-1)/2$ *regular* terms, which is too expensive in the general case. This was eventually solved by introducing an additional equation of motion for the change in the two-body energy due to perturbations. Thus by the time of IAU Colloquium 10 on the N-body problem in 1970 two general codes were presented which included KS regularization [Aarseth, 1972b; Bettis & Szebehely, 1972]. Sadly, the latter proved too expensive for large systems since it employed a high-order Runge–Kutta integrator and was not developed further. However, it did prove itself in an investigation of high-velocity escapers in small systems [Allen & Poveda, 1972].

On the personal front, the next few years saw some interesting applications. One collaboration adopted hierarchical initial conditions inspired by fragmentation theory [Aarseth & Hills, 1972], which led to some energetic interactions. It is now well established that very young clusters show evidence of subclustering. Another effort examined the depletion of low-mass stars and concluded that the preferential effect was somewhat less than expected on theoretical grounds [Aarseth & Wolf, 1972]. The question of energetic binaries halting core collapse was also discussed [Aarseth, 1972a]. It was shown that a central binary may acquire a

[§] The treatment of mixed secular terms was later improved by Mikkola [1984a] who introduced the variation of the epoch.

significant fraction of the total energy even for systems with $N = 500$; a calculation that took some 500 hours to complete [Aarseth, 1974]. It is noteworthy that the dominant binary acquired 50% of the total energy after only 12 crossing times (defined in the next section). Finally, a small contribution contained the first simulation of what we now call primordial binaries [Aarseth, 1975], which has become a major industry.¶

The 1970s brought about two important technical developments which are still being used. First we mention the Ahmad–Cohen [1973] neighbour scheme. The basic idea here is to represent the force acting on a particle by a sum of two polynomials, with the neighbour contribution being updated more frequently. Although there are programming complications due to the change of neighbours, the method is truly collisional and speeds up the calculation significantly even for quite modest values of N. Before the advent of the HARP special-purpose computer (to be described later), this algorithm facilitated the simulation of larger cluster models with $N \simeq 10^4$ where the gain may be a factor of 10.

The second innovation occurred by a happy combination of circumstances which resulted in a three-body regularization method [Aarseth & Zare, 1974]. This was achieved by the introduction of two coupled KS solutions which permit two of the particle pairs to approach each other arbitrarily close, provided this does not take place simultaneously. It turns out that the third interaction modifies the equations of motion in a way that still maintains regularity, as long as the corresponding distance is not the smallest. Following this development, the global formulation by Heggie [1974] was a notable achievement, especially since it was generalized to the N-body problem.

It is perhaps surprising that, for practical purposes, the algorithm based on two separable KS solutions is preferable to the global regularization for $N = 3$. However, the treatment of just four particles in a similar way had to wait for a technical simplification, eventually conceived by Mikkola [1985a].‖ In the event, the Ahmad–Cohen method was combined with standard KS as well as the *unperturbed* three- and four-body regularization methods to form the embryonic NBODY5 code towards the end of the 1970s. Right from the start, the KS treatment was generalized to an arbitrary number of simultaneous particle pairs, necessitating a considerable amount of automatic decision-making.

A comparison of the multiple regularization methods has been carried out for $N = 3$ and $N = 4$ [Alexander, 1986], whereas a general review of integration methods for few-body systems is also available [Aarseth, 1988a]. An early study of core collapse for $N = 1000$ illustrated the

¶ The study of initial hard binaries was urged in the thesis of Heggie [1972b].

‖ The early history of multiple regularization has been recorded by Mikkola [1997b].

usefulness of the new techniques [Aarseth, 1985b]. Finally, we mention a pioneering development of a hybrid code which combined the Fokker–Planck method with direct integration and KS regularization [McMillan & Lightman, 1984a,b].

We end this historical review by noting that ideas for increasing the speed of the calculation were discussed at an early stage [Aarseth & Hoyle, 1964]. At that time an increase in the particle number from 100 to 300 seemed to be the practical limit based on an argument that gave the computing time proportional to N^3 for a given degree of evolution. This analysis also anticipated subsequent developments of introducing a collisionless representation in order to reach much larger values of N. It was estimated that a shell method with up to five spherical harmonics would allow $N \simeq 5000$ to fit the current maximum memory of 64 K.

Modern times have seen some significant advances, both as regards software and hardware. The N-body problem has matured and we are now entering an exciting new area. In this spirit we leave history behind and will attempt to discuss a variety of relevant N-body developments in subsequent chapters.

1.3 Basic concepts

In this book, we are primarily interested in applications of the original Newton's Law of Gravity, as opposed to a modified expression including softening. The equations of motion for a particle of index i in a system containing N particles then take the form

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1;\, j=i}^{N} \frac{m_j(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} \,. \tag{1.1}$$

For convenience, we use scaled units in which $G = 1$ and define the left-hand side of (1.1) as the force *per unit mass*, $\mathbf{F}_i$. Given the initial conditions $m_i, \mathbf{r}_i, \mathbf{v}_i$ for the mass, coordinates and velocity of each particle at some instant t_0, the set of $3N$ second-order differential equations (1.1) then defines the solutions $\mathbf{r}_i(t)$ over the time interval $(-\infty, \infty)$. Alternatively, the complete solutions are also specified by $6N$ first-order equations that must be solved in a self-consistent manner, and the latter procedure is in fact usually chosen in practice.

It has been known since Newton's days that the *N-body problem* defined by (1.1) only admits exact solutions for the case of two interacting particles. All that is known with certainty beyond this is that there exist ten integrals of the motion. For completeness, let us introduce these fundamental relations which are often used as a check on accuracy. The total

energy and angular momentum (E and $\mathbf{J}$) of the system are defined by

$$E = \frac{1}{2}\sum_{i=1}^{N} m_i \mathbf{v}_i^2 - \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{G m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}\,, \tag{1.2}$$

$$\mathbf{J} = \sum_{i=1}^{N} \mathbf{r}_i \times m_i \mathbf{v}_i\,. \tag{1.3}$$

The two terms of (1.2) represent the total kinetic and potential energy, respectively. Multiplying (1.1) by m_i and performing a summation, we obtain

$$\sum_{i=1}^{N} m_i \ddot{\mathbf{r}}_i = 0 \tag{1.4}$$

by symmetry. Integrating, we find that in the absence of any external forces the centre of mass of the system moves with constant velocity, thus providing an additional six conserved quantities. The demonstration that the total energy and angular momentum are also constant can be left as an exercise [see e.g. Roy, 1988, pp.113–115 for proofs]. We define T, U, W as the total kinetic, potential and external energy, with $U < 0$. The basic energy relation then takes the more general and compact form

$$E = T + U + W\,, \tag{1.5}$$

which is convenient for discussions. Another quantity useful for numerical algorithms is the Lagrangian energy,

$$L = T - U\,, \tag{1.6}$$

although the positive sign convention for U is often chosen here.

From the above, it follows that a good numerical scheme for conservative systems needs to maintain satisfactory values for the ten constants of the motion during all times of interest. Unfortunately, errors are always present in any step-wise scheme (as in the simplest numerical computation), hence we speak about the *deviation* from the initial values instead. Since the total energy is the difference between two large numbers, T and $|U|$, experience has shown that this is the most sensitive quantity for monitoring the accuracy. However, if we are unlucky, the errors might still conspire in such a way as to cancel and thereby render energy conservation meaningless. Yet, the general tendency is for such errors to be systematic and hence more readily identified. In order to make progress beyond the basic scheme outlined above, we shall simply take a positive attitude towards obtaining numerical solutions and delay a fuller discussion of this difficult subject until later.

The crossing time is undoubtedly the most intuitive time-scale relating to self-gravitational systems. For a system in approximate dynamical equilibrium it is defined by

$$t_{\rm cr} = 2\,R_{\rm V}/\sigma\,, \tag{1.7}$$

where $R_{\rm V}$ is the virial radius, obtained from the potential energy by $R_{\rm V} = GN^2\bar{m}^2/2|U|$, and σ is the rms velocity dispersion. In a state of approximate equilibrium, $\sigma^2 \simeq GN\bar{m}/2R_{\rm V}$, which gives

$$t_{\rm cr} \simeq 2\sqrt{2}\,(R_{\rm V}^3/GN\bar{m})^{1/2}\,, \tag{1.8}$$

with $\bar{m}$ the mean mass, or alternatively $t_{\rm cr} = G(N\bar{m})^{5/2}/(2|E|)^{3/2}$ from $E = \frac{1}{2}U$. Unless the total energy is positive, any significant deviation from overall equilibrium causes a stellar system to adjust globally on this time-scale which is also comparable to the free-fall time. The close encounter distance is a useful concept in collisional dynamics. It may be defined by the expression [Aarseth & Lecar, 1975]

$$R_{\rm cl} = 2\,G\bar{m}/\sigma^2\,, \tag{1.9}$$

which takes the simple form $R_{\rm cl} \simeq 4\,R_{\rm V}/N$ at equilibrium.

Since much of this book is devoted to star clusters, it may be instructive to introduce some basic parameters for clusters to set the scene for the subsequent numerical challenge. A rich open star cluster may be characterized by $N \simeq 10^4$, $\bar{m} \simeq 0.5\,M_\odot$ and $R_{\rm V} \simeq 4\,{\rm pc}$, which yields $t_{\rm cr} \simeq 5 \times 10^6\,{\rm yr}$. Many such clusters have ages exceeding several Gyr, hence a typical star may traverse or orbit the central region many times, depending on its angular momentum. Another relevant time-scale in N-body simulations is the orbital period of a binary. Let us consider a typical close binary with separation $a \simeq R_{\rm V}/N$. With a period of $\simeq 700\,{\rm yr}$ this would make some 7000 orbits in just one crossing time. Thus, in general, if $a = fR_{\rm V}/N$ there would be $\simeq N/f^{3/2}$ Kepler orbits per crossing time.

The subject of relaxation time is fundamental and was mainly formulated by Rosseland [1928], Ambartsumian [1938, 1985], Spitzer [1940] and Chandrasekhar [1942]. The classical expression is given by

$$t_{\rm E} = \frac{1}{16}\left(\frac{3\pi}{2}\right)^{1/2}\left(\frac{NR^3}{Gm}\right)^{1/2}\frac{1}{\ln(0.4N)}\,, \tag{1.10}$$

where R is the size of the homogeneous system [Chandrasekhar, 1942]. For the purposes of star cluster dynamics, the half-mass relaxation time is perhaps more useful since it is not sensitive to the density profile.

Following Spitzer [1987], it is defined by**

$$t_{\rm rh} = 0.138 \left(\frac{N r_{\rm h}^3}{Gm} \right)^{1/2} \frac{1}{\ln(\gamma N)} , \tag{1.11}$$

where $r_{\rm h}$ is the half-mass radius and $\Lambda = \gamma N$ is the argument of the Coulomb logarithm. Formally this factor is obtained by integrating over all impact parameters in two-body encounters, with a historical value of $\gamma = 0.4$. Some of the most important subsequent determinations are due to Hénon [1975] and Giersz & Heggie [1994a], who obtained the respective values 0.15 and 0.11 for equal masses, with the latter derived from numerical measurements. Although this factor only enters through the term $\ln(\gamma N)$, it can still make a significant difference in numerical comparisons which are now becoming quite reliable when using ensemble averages. As the second authors point out, the corresponding value for a general mass spectrum is reduced considerably. From the numerical example above we then have $t_{\rm rh} \simeq 3 \times 10^8$ yr for $r_{\rm h} \simeq 4$ pc and an equal-mass system with $N = 1 \times 10^4$ stars of half a solar mass. In comparison, $t_{\rm rh} \simeq 3 \times 10^{10}$ yr for a globular cluster with $N \simeq 10^6$ and $r_{\rm h} \simeq 25$ pc.

An alternative viewpoint on the derivation of the two-body relaxation time is promoted in the review by Spurzem [1999]. Based on the pioneering work of Larson [1970] which was continued by Louis & Spurzem [1991] and Giersz & Spurzem [1994], the collisional term in the Fokker–Planck description can be developed to yield unambiguous expressions for the classical types of relaxation discussed here. Now the relaxation time emerges naturally as the consequence of the interaction of two distribution functions and the choice of their form as well as that of the Coulomb logarithm uniquely determines the nature of the different processes. Thus instead of assuming the usual small angle deflections of the orbit, it is inferred directly that the Coulomb integral starts at an angle of 90 .

The expression (1.11) gives an estimate of the time for the rms velocity change arising from small angle deflections at the half-mass radius to become comparable to the initial velocity dispersion. It serves as a useful reference time for significant dynamical changes affecting the whole cluster even though there is no corresponding numerically well-defined quantity. The assumption of approximate equilibrium with the above definition of the crossing time leads to the relation [Spitzer, 1987]

$$\frac{t_{\rm rh}}{t_{\rm cr}} \simeq \frac{N}{22 \, \ln(\gamma N)} , \tag{1.12}$$

which shows that close encounters become less important for increasing particle number since the potential is smoother. Hence if the relaxation

** Also see Spitzer & Hart [1971a] for an alternative derivation.

time for an equal-mass system exceeds the time interval of interest by a significant factor, the use of the collisionless approximation which neglects close encounters may be justified. However, the approach to the collisionless regime is slow and in any case the central relaxation time may be much shorter.

An equivalent formulation of the relaxation time in terms of the deflection angles suffered by a test star yields comparable values to (1.10) [Williamson & Chandrasekhar, 1941]. This expression has in fact been tested numerically for different velocities [Lecar & Cruz-González, 1972] and particle numbers $N \leq 2500$ [Aksnes & Standish, 1969], providing agreement with theory on the assumption of independent individual encounters.

The concept of dynamical friction was introduced by Chandrasekhar [1942] who elucidated the tendency for a star to be decelerated in the direction of its motion. This refinement reconciled the predicted escape rate with the possible presence of some old open clusters. However, the analysis was not extended to the case of massive stars which later merited considerable interest with the emphasis on mass segregation in stellar systems. In the case of a slow-moving body of mass $m_2 \gg \bar{m}$ but within 20 % of the total mass, the frictional force can be written in the simplified form [Binney & Tremaine, 1987]

$$\frac{d\mathbf{v}_2}{dt} = -\frac{4\pi \ln \Lambda G^2 \rho m_2}{v_2^3} \left[\mathrm{erf}(X) - \frac{2X}{\sqrt{\pi}} \exp(-X^2) \right] \mathbf{v}_2 \,, \tag{1.13}$$

where ρ is the background density and $X = v_2/(2\sigma)^{1/2}$.

Rich star clusters are usually centrally concentrated, with an extended halo. The majority of central stars are strongly bound and therefore experience changes in their orbital elements on shorter time-scales than given by (1.11). A corresponding mean relaxation time can be derived by integrating the general expression [e.g. Chandrasekhar, 1942] for a given cluster model. This was done a long time ago for polytropic models, increasing the classical value by a factor of 4 in the case of $n = 5$ [King, 1958]. On the other hand, the central relaxation time can be much shorter for realistic models with high central densities. This runaway process called core collapse (and its aftermath) has fascinated theoreticians and will be discussed further in another chapter. Let us just remark that the formation of a bound halo, together with a small fraction of escaping particles, is a direct consequence of this process by virtue of energy conservation. In short, the evolution takes place because there is no equilibrium.

So far we have mainly considered equal-mass systems, which are more amenable to analytical treatment and have therefore attracted more attention. However, the general case of a mass spectrum is more relevant for