Gravitational N-Body Simulations

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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].

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* The story of how it all began is told in von Hoerner [2001]. Also of historical interest is the early study of gravitational interactions between two model galaxies based on measuring the intensity of 37 light bulbs at frequent intervals [Holmberg, 1941]. Finally, a general three-body integration by Strömgren [1900, 1909] was carried out by hand, albeit for only part of an orbit. More than 100 years ago he anticipated that the method of 'mechanical integration' may be extended to deal with four or more bodies and be of considerable importance for the theory of stellar systems.

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.

[†] The method of individual time-steps was originally suggested by A. Schlüter [private communication, 1961].

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 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.

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

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

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 *NBODY*5 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 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].

¶ 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].

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

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

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 $R_{\rm V} \simeq 4\,$pc, which yields $t_{\rm cr} \simeq 5 \times 10^6\,$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 $\simeq 700\,$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[**]

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

where r_{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 $t_{\mathrm{rh}} \simeq 3 \times 10^8$ yr for $r_{\mathrm{h}} \simeq 4$ pc and an equal-mass system with $N = 1 \times 10^4$ stars of half a solar mass. In comparison, $t_{\mathrm{rh}} \simeq 3 \times 10^{10}$ yr for a globular cluster with $N \simeq 10^6$ and $r_{\mathrm{h}} \simeq 25$ 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]

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

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

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[**] 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]

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

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 star cluster simulations. The time-scale associated with some aspects of mass segregation is probably better determined than the relaxation times above. Analysis of a two-component system dominated by light particles gave rise to the equipartition time for kinetic energy [Spitzer, 1969]

$$t_{\rm eq} = \frac{(\bar{v}_1^2 + \bar{v}_2^2)^{3/2}}{8(6\pi)^{1/2} G^2 \rho_{01} m_2 \ln N_1}\,, \qquad (1.14)$$

where ρ_{01} is the central density of the N_1 light stars of mass m_1. It is envisaged that the heavy particles of mass m_2 lose kinetic energy through encounters with lighter particles of mass m_1 and spiral inwards.

The expression above holds, provided that the heavy particles do not form a self-gravitating system, in which case standard relaxation takes over. The equipartition condition is expressed in terms of the corresponding total masses as $M_2/M_1 < \beta(m_1/m_2)^{3/2}$, where $\beta \simeq 0.16$ for large mass ratios. After a phase of contraction the heavy particles begin to form a self-gravitating system and the evolution rate slows down. To the extent that the expression (1.14) is applicable, it can be seen that the presence of a mass spectrum speeds up the early evolution. Hence, in general, we have that $t_{\rm eq} \simeq t_{\rm E}\bar{m}/m_2$ for the case of two unsegregated populations with comparable velocity dispersions [Spitzer, 1969]. Comprehensive theoretical discussions of time-scales and evolution processes in rich star clusters can be found in several reviews [Meylan & Heggie, 1997; Gerhard, 2000]. However, we emphasize that as yet there is no consistent theory of the relaxation time for a realistic IMF.

Although most old clusters are in a state of approximate virial equilibrium, this may not be the case for very young clusters. Non-equilibrium initial conditions are often chosen in simulations in order to model systems with significant mass motions. Some early simulations that employed a spherical shell model demonstrated that collisionless systems reach overall equilibrium on a relatively short time-scale [Hénon, 1964, 1968]. The concept of *violent relaxation* [Lynden-Bell, 1967] was introduced to describe galaxy formation but is equally relevant for star clusters. Before making some general comments, let us write the virial theorem in the traditional scalar form [Chandrasekhar, 1942, p.219; Fukushige & Heggie, 1995]

$$d^2I/dt^2 = 4T + 2U + 4A - 4W\,, \qquad (1.15)$$

where I is the moment of inertia and A represents the angular momentum contribution, $\Omega_z J_z$, for cluster motion in the Galactic plane with angular velocity Ω_z. Hence in this case the virial ratio is defined by

$$Q_{\rm vir} = (T + A)/|U - 2W|)\,. \qquad (1.16)$$

Setting $A = 0$ and $W = 0$ for simplicity and choosing initial velocities, collapse takes place if $Q_{\rm vir} < 0.5$, with enhanced mass motions for small values.

A qualitative description of the collapse phase may be made by considering the energy per unit mass of a particle,

$$E_i = \tfrac{1}{2}\mathbf{v}_i^2 + \Phi_i \,, \tag{1.17}$$

with velocity $\mathbf{v}_i$ and potential Φ_i. In the extreme case of starting from rest, all the particles move inwards on radial orbits. These orbits are perturbed by neighbouring particles, acquiring angular momentum. This leads to a dispersion in the collapse times, even for a homogeneous system. Consequently, the early arrivals are decelerated in their outward motion, whereas the late-comers experience a net acceleration. Following the bounce, the core–halo system may also have a significant fraction of particles with positive energy that subsequently escape. The initial collapse therefore leads to a considerable redistribution of the binding energies and the system undergoes violent relaxation. An early investigation of homogeneous N-body systems starting from rest [Standish, 1968a] showed that about 15% of the particles gained enough energy to escape. A variety of one-dimensional experiments made at the time also confirmed that an equilibrium distribution is only reached for the inner part [Lecar & Cohen, 1972].

A much more careful analysis is needed to provide a detailed description of even the simplest collapsing system and is beyond the present scope [Aarseth, Lin & Papaloizou, 1988]. However, it is worth emphasizing that such systems can be studied by numerical methods, which may be used to test theoretical ideas. In the present context, violent relaxation is assumed to be collisionless and is therefore only applicable in the limit of large N. However, the general process is also effective in systems with $N = 500$ which are in fact subject to mass segregation at the same time [Aarseth & Saslaw, 1972; Aarseth, 1974].

Following on from non-equilibrium systems, the analogy with an eccentric binary illustrates some aspects relating to the virial theorem. Consider a plot of the virial ratio, $Q_{\rm vir}$, for collapsing systems that shows several oscillations of decreasing amplitude about the equilibrium value $\bar{Q}_{\rm vir} = 0.5$ [Standish, 1968a].[††] However, small fluctuations are still present even after many crossing times. This behaviour can be understood by examining an isolated binary. Taking the ratio of kinetic and potential energy leads to the simple expression

$$Q_{\rm vir} = 1 - R(t)/2a \,, \tag{1.18}$$

[††] We are not concerned with the excess of kinetic energy due to escaping particles.

where $R(t)$ is the instantaneous separation. Hence an eccentric binary exhibits a varying virial ratio which depends on the phase and eccentricity. Now let such an energetic binary be part of the system. Even if its energy is constant, the contribution to the virial ratio may dominate the whole system near an eccentric pericentre. Needless to say, this feature is not of dynamical significance and because of the special treatment of binaries in the present formulation, such contributions are not included here.

Star clusters orbiting the Galaxy are subject to an external tidal field which tends to increase the disruption rate. In this connection we introduce the classical concept of tidal radius [von Hoerner, 1957; King, 1962]. The simple picture of the tidal radius is that stars that move outside this distance escape from the cluster on a relatively short time-scale. However, actual orbit calculations show that the situation is more complicated even for clusters in circular orbits [Ross, Mennim & Heggie, 1997; Heggie, 2001]. In the case of globular clusters, the process of tidal shocks also needs to be modelled [Ostriker, Spitzer & Chevalier, 1976; Spitzer, 1987].

According to theory, close encounters act to maintain a Maxwellian velocity distribution in equilibrium systems. Thus after one relaxation time, a fraction $Q_{\rm e} \simeq 0.007$ should exceed the escape velocity in an isolated system [Chandrasekhar, 1942] and then be replenished. When discussing escape from stellar systems, we distinguish between ejection due to one close encounter [Hénon, 1969] and evaporation, caused by the cumulative effect of many weak encounters. From general considerations, the former outcome declines in importance with increasing N for systems dominated by single stars, whereas the presence of binaries complicates the issue. Although the process of escape is fundamental, the complexity of the interactions is such that only general statements can be made, especially when different masses are involved. For example, classical theory states that equipartition of kinetic energy will be achieved on a time-scale $t_{\rm eq}$ which is comparable to $t_{\rm rh}$ for $N \simeq 100$ and modest mass ratios. A moment's reflection is enough to show that this argument is fallacious.

In self-gravitating systems the central escape velocity is some factor, $f_{\rm e} \geq 2$, times the rms velocity, where the actual value depends on the density profile. Consequently, the equipartition condition $mv^2 = \text{const}$ can only be satisfied for modest mass ratios, beyond which escape invariably occurs. What actually happens is that the lighter particles occupy a larger volume and hence their relaxation time increases. A better way to look at energy equipartition is to compare $m\bar{v}^2$ for certain mass groups at similar central distances, rather than globally. In any case, the tendency for massive particles to be preferentially concentrated in the central region is a direct consequence of the equipartition process, whereby the loss of kinetic energy leads to inward spiralling [Aarseth, 1974]. These simple considerations show that although theoretical concepts are very useful for a general understanding of dynamics, numerical solutions can often obtain a more consistent picture, albeit for limited particle numbers.

1.4 The first steps

The well-known saying about learning to walk before you can run is highly appropriate for the aspiring N-body simulator, since much play is made of making runs. Hence we start our Odyssey at the most primitive stage in order to illustrate the main principles involved for performing direct numerical integrations.

In order to obtain numerical solutions, we proceed by advancing all coordinates and velocities using sufficiently small intervals, re-evaluating the accelerations by the summation (1.1) after each increment. At the most primitive level we can relate the solutions at time t to the previous solution at time t_0 by a Taylor series expansion to lowest order as

$$\begin{aligned} \mathbf{v}_i(t) &= \mathbf{F}_i \Delta t + \mathbf{v}_i(t_0)\,, \\ \mathbf{r}_i(t) &= \tfrac{1}{2}\mathbf{F}_i \Delta t^2 + \mathbf{v}_i(t_0)\Delta t + \mathbf{r}_i(t_0)\,, \end{aligned} \tag{1.19}$$

where $\Delta t = t - t_0$ is a suitably chosen small time interval and $\mathbf{F}_i$ is evaluated by (1.1) at $t = t_0$. From dimensional considerations, we require that $|\mathbf{v}_i|\Delta t \ll r_{\rm h}$ for meaningful results. A complete solution then involves advancing (1.19) simultaneously for all the particles until some specified condition has been satisfied. This step-by-step method (standard Euler) is clearly very laborious since each force summation includes $O(N)$ operations and Δt needs to be small in order to maintain a reasonable accuracy. However, it does contain the basic idea of obtaining self-consistent solutions for the set of coupled differential equations (1.1).

Numerical solutions of equations (1.19) are readily obtained for the two-body problem. Choosing a circular binary, we find a relative error of the semi-major axis *per orbit* of $\Delta a/a \simeq 8 \times 10^{-3}$ when averaged over ten initial periods. Here the time-step was chosen according to $2\pi\eta R^{3/2}$ from Kepler's Law, with $\eta = 0.0002$, which gives 5000 steps for each revolution.

The errors reduce dramatically by going to the improved Euler method. First provisional coordinates are predicted in the usual way by

$$\tilde{\mathbf{r}}_i(t) = \tfrac{1}{2}\mathbf{F}_i \Delta t^2 + \mathbf{v}_i(t_0)\Delta t + \mathbf{r}_i(t_0)\,, \tag{1.20}$$

whereupon the new force, $\mathbf{F}_i(t)$, is obtained from (1.1). We define the average force during the interval Δt as

$$\bar{\mathbf{F}}_i = \tfrac{1}{2}\left[\mathbf{F}_i(t) + \mathbf{F}_i(t_0)\right] . \tag{1.21}$$

The average force is then used to calculate the final values of $\mathbf{v}_i(t)$ and $\mathbf{r}_i(t)$ according to (1.19). Now we obtain $\Delta a/a \simeq -6 \times 10^{-9}$ per revolution, whereas $\eta = 0.002$ gives $\Delta a/a \simeq -6 \times 10^{-6}$, which is considerably more accurate than the standard Euler method above for ten times as many steps. Eccentric orbits require more integration steps because of the smaller pericentre distance and also produce somewhat larger errors. Thus in the case of the improved Euler method an eccentricity $e = 0.75$ leads to $\Delta a/a \simeq -4 \times 10^{-5}$ per revolution with $\eta = 0.002$.

This simple exercise demonstrates an important aspect about numerical integrations, namely that the accuracy may be improved significantly by making better use of existing information at small extra cost. In view of the expensive summation (1.1) for large N, it is worth emphasizing that the improved scheme also uses only one force evaluation per step. This desirable property is exploited in the more sophisticated developments discussed below and in the next chapter.

After illustrating the general principles of direct N-body integration, it may be appropriate to present the basic integration method of von Hoerner [1960] since it is not available in the English literature. For historical reasons, we retain the original notation which does not use vectors. Denoting the coordinates and velocity of a particle i by $x_{\alpha i}$ and $u_{\alpha i}$, respectively, with $\alpha = 1, 2, 3$, the coupled equations of motion for a system of equal masses take the form

$$\begin{aligned} \frac{dx_{\alpha i}}{dt} &= u_{\alpha i}\,, \\ \frac{du_{\alpha i}}{dt} &= -Gm \sum_{j=1;\, j\neq i}^{N} \frac{x_{\alpha i} - x_{\alpha j}}{r_{ij}^3}\,, \end{aligned} \tag{1.22}$$

where r_{ij} is the mutual separation. The original derivation adopted the scaling $Gm = 1$ for equal-mass systems but in any case the following discussion is general.

The new time-step is determined from the closest particle pair by taking the harmonic mean of the travel time, $\tau_1 = D_\mathrm{m}/V_\mathrm{m}$, and free-fall time, $\tau_2 = D_\mathrm{m}(2D_\mathrm{m})^{1/2}$, according to

$$h_2 = \frac{D_\mathrm{m}(2D_\mathrm{m})^{1/2}}{\mu\left[1 + V_\mathrm{m}(2D_\mathrm{m})^{1/2}\right]}\,. \tag{1.23}$$

Here D_m is the minimum separation, V_m the corresponding relative velocity and μ is an accuracy parameter. Consider the system at an epoch $t_0 = 0$, with h_1 the previous step. Moreover, let u_1 and x_1 denote the velocity at $-\frac{1}{2}h_1$ and coordinates at t_0, respectively, where the subscripts have been omitted for clarity. Assuming a linear dependence over the interval $[-h_1, h_2]$, we write the force as

$$b = b_1 + a_1 t\,, \tag{1.24}$$

where $a_1 = (b_1 - b_0)/h_1$ is the divided force difference over the previous interval, $[-h_1, 0]$. After some algebra we obtain the predicted velocity and coordinates

$$\begin{aligned} u_2^0 &= u_1 + k_0 b_1 + k_2 a_1\,, \\ x_2^0 &= x_1 + h_2 u_2^0 + k_1 a_1\,, \end{aligned} \tag{1.25}$$

with the coefficients $k_0 = \frac{1}{2}(h_2 + h_1)$, $k_1 = \frac{1}{24}h_2^3$ and $k_2 = \frac{1}{8}(h_2^2 - h_1^2)$.

The solution can be improved after calculating the new force, b_2, at $t = h_2$. This is achieved[‡‡] by writing a parabolic force fitting function as

$$b = b_1 + a_1 t + d_2(h_1 t + t^2)/(h_2 + h_1)\,. \tag{1.26}$$

Setting $b = b_2$ at the end of the interval h_2 simplifies to

$$d_2 = (b_2 - b_1)/h_2 - a_1\,. \tag{1.27}$$

The contributions from the last term of (1.26) can now be included to yield the corrected solutions for u_2 at $t = h_2/2$ and x_2 at $t = h_2$,

$$\begin{aligned} u_2 &= u_2^0 + k_3 d_2\,, \\ x_2 &= x_2^0 + k_5 d_2\,, \end{aligned} \tag{1.28}$$

where[§§] $k_3 = \frac{1}{24}(h_2^2 + 2h_2 h_1 - 2h_1^2)$ and $k_5 = \frac{1}{12}h_2(h_2^2 + h_2 h_1 - h_1^2)$.

The employment of a leapfrog method gives rise to enhanced stability for a given integration order [cf. Hut, Makino & McMillan, 1995]. However, the question of the initial velocity requires special attention. Thus it is advantageous to choose a conservative initial step, h_1, and integrate backwards an interval $\Delta t = -\frac{1}{2}h_1$ before beginning the calculation. The subsequent few time-steps, h_2, may then be restricted to grow by a small factor to ensure convergence of the force polynomials. Special care is also needed for evaluating the total energy, since the velocities are known at $t - \frac{1}{2}h_2$ and it is desirable to attain the highest accuracy consistently. Thus for the purpose of calculating the kinetic energy at the end of the current time-step, h_2, the predicted velocity is obtained by integrating (1.26) over $[h_2/2,\ h_2]$ and adding u_2 which finally gives

$$u = u_2 + b_1 h_2/2 + 3a_1 h_2^2/8 + d_2 h_2^2(3h_1/8 + 7h_2/24)/(h_2 + h_1)\,. \tag{1.29}$$

[‡‡] The so-called ‘semi-iteration’ was also proposed by A. Schlüter [cf. von Hoerner, 1960].

[§§] Corrected for a typographical error in the last term of k_3.

Table 1.1. Integration errors with von Hoerner's method.

N	Steps	$t/t_{\rm cr}$	μ	$\Delta E/E$	ΔJ_z	$a_{\rm min}$
16	6200	5	6	1×10^{-4}	2×10^{-7}	0.046
16	8800	5	10	9×10^{-6}	3×10^{-8}	0.080
16	18 000	10	6	2×10^{-4}	4×10^{-7}	0.022
25	10 000	5	10	1×10^{-6}	1×10^{-8}	0.029
25	16 000	5	20	5×10^{-8}	1×10^{-9}	0.086
25	127 000	10	20	7×10^{-6}	2×10^{-9}	0.007

Unless there are long-lived binaries with short period, test calculations generally give satisfactory energy errors when using $\mu = 10$.

It is instructive to compare von Hoerner's method for the two-body example discussed above. The eccentric orbit with $e = 0.75$ and $\eta = 0.002$ now gives $\Delta a/a \simeq -1.3\times10^{-5}$ per revolution for the case of semi-iteration. This improves to $\simeq -3\times10^{-7}$ when the corrector (1.28) is included. Hence the first N-body method is superior to the improved Euler method for the same number of steps per orbit.

A more general comparison test has also been performed. The initial conditions are generated in the same way as the original paper, which employed virialized velocities inside a homogeneous sphere of radius 1 and $m = 1$. All the calculations are carried out with standard double precision. Table 1.1 gives some characteristic values of relative energy errors and change in the angular momentum about the z-axis for intervals of $0.2t_{\rm cr}$. All deviations are measured with respect to initial values and the last column shows the smallest semi-major axis. Although the relative energy errors are satisfactory in these examples, the presence of a highly eccentric binary introduces a noticeable systematic orbital shrinkage which is expensive to counteract with the present basic treatment.

The device of including the semi-iteration (or corrector) without recalculating the force improves the solutions by almost one full order. It was also adopted in subsequent formulations[¶¶] based on high-order force polynomials [cf. Wielen, 1967, 1972; Aarseth, 1968] with $N \leq 250$, whereas the original calculations were performed with up to 16 equal-mass particles. The choice of accuracy parameter $\mu = 6$ led to maximum relative energy errors $\Delta E/E \simeq 4 \times 10^{-3}$ for $t \simeq 9\,t_{\rm cr}$ in spite of only about ten figure machine accuracy combined with a relatively low order. However, the very first general N-body simulation already produced some interesting information on topics such as relaxation time, binary formation and escape that have stood up to the test of time.

[¶¶] Already included in a third-order polynomial scheme for $N = 100$ [Aarseth, 1966a].