2

Predictor–corrector methods

2.1 Introduction

In this chapter, we provide the tools needed for standard N-body integration. We first review the traditional polynomial method which leads to increased efficiency when used in connection with individual time-steps. This self-contained treatment follows closely an earlier description [Aarseth, 1985a, 1994]. Some alternative formulations are discussed briefly for completeness. We then introduce the simpler Hermite scheme [Makino, 1991a,b] that was originally developed for special-purpose computers but is equally suitable for workstations or laptops and is attractive by its simplicity. As discussed in a later section, the success of this scheme is based on the novel concept of using quantized time-steps (factor of 2 commensurate), which reduces overheads. Variants of the Hermite method were attempted in the past, such as the low-order scheme of categories [Hayli, 1967, 1974] and the full use of explicit Taylor series derivatives [Lecar, Loeser & Cherniack, 1974]. The former study actually introduced the idea of hierarchical time-steps with respect to individual force calculations using a low-order scheme, whereas the latter formulation is expensive (but accurate) even for modest particle numbers.

2.2 Force polynomials

The force acting on a particle usually varies in a smooth manner throughout an orbit, provided the particle number is sufficiently large. Hence by fitting a polynomial through some past points, it is possible to extend the time interval for advancing the equations of motion and thereby reduce the number of force evaluations. In other words, we can use the past information to predict the future motion with greater confidence. Such a scheme was already introduced in the pioneering work of von Hoerner

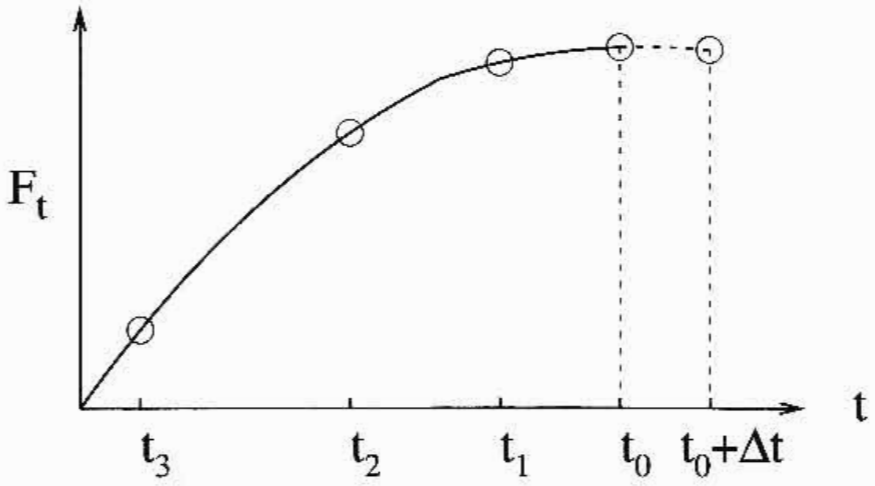

Fig. 2.1. Force polynomial fitting.

[1960], who adopted a quadratic interpolation of the force on each particle. In the following years formulations based on higher orders were employed [Aarseth, 1966a, 1968; Wielen, 1967]. Experience has shown that there is some gain in increasing the order of the integration scheme but the law of diminishing returns applies and it appears that four orders is sufficient for most purposes [Wielen, 1967, 1974]. A subsequent investigation [Makino, 1991a] showed that the fourth-order scheme* is within 30% of the minimum cost for all values of the rms energy error. The present difference formulation is based on the notation of Ahmad & Cohen [1973; hereafter AC] and follows closely an earlier treatment [Aarseth, 1985a]. In the subsequent description we omit the particle subscript in $\mathbf{F}_i$ and related quantities for clarity.

On some time-scale, the force on a particle can be considered to be smoothly varying, as illustrated by Fig. 2.1, and can therefore be approximated by a continuous function. Given the values of $\mathbf{F}$ at four successive past epochs t_3, t_2, t_1, t_0, with t_0 the most recent, we write a fourth-order fitting polynomial at time t valid in the interval $[t_3, t_0 + \Delta t]$ as

$$\mathbf{F}_t = \left\{ \left[\left(\mathbf{D}^4(t - t_3) + \mathbf{D}^3 \right) (t - t_2) + \mathbf{D}^2 \right] (t - t_1) + \mathbf{D}^1 \right\} (t - t_0) + \mathbf{F}_0 \,. \tag{2.1}$$

Using compact notation, the first three divided differences are defined by

$$\mathbf{D}^k[t_0, t_k] = \frac{\mathbf{D}^{k-1}[t_0, t_{k-1}] - \mathbf{D}^{k-1}[t_1, t_k]}{t_0 - t_k} \,, \qquad (k = 1, 2, 3) \tag{2.2}$$

where $\mathbf{D}^0 \equiv \mathbf{F}$ and square brackets refer to the appropriate time intervals, such that $\mathbf{D}^2[t_1, t_3]$, for instance, is evaluated at t_1. The term $\mathbf{D}^4$ is defined similarly by $\mathbf{D}^3[t, t_2]$ and $\mathbf{D}^3[t_0, t_3]$.

* This is two orders more than used by von Hoerner but one order less than Wielen.

Conversion of the force polynomial into a Taylor series provides simple expressions for integrating the coordinates and velocities. Equating terms in the successive time derivatives of (2.1) with an equivalent Taylor series and setting $t = t_0$ yields the corresponding force derivatives

$$\begin{aligned}
\mathbf{F}^{(1)} &= [(\mathbf{D}^4 t_3' + \mathbf{D}^3)t_2' + \mathbf{D}^2]t_1' + \mathbf{D}^1 , \\
\mathbf{F}^{(2)} &= 2![\mathbf{D}^4(t_1't_2' + t_2't_3' + t_1't_3') + \mathbf{D}^3(t_1' + t_2') + \mathbf{D}^2] , \\
\mathbf{F}^{(3)} &= 3![\mathbf{D}^4(t_1' + t_2' + t_3') + \mathbf{D}^3] , \\
\mathbf{F}^{(4)} &= 4!\mathbf{D}^4 ,
\end{aligned} \tag{2.3}$$

where $t_k' = t_0 - t_k$. These equations are mainly used to obtain the Taylor series derivatives at $t = t_0$, when the fourth difference is not yet known. Thus the contribution from $\mathbf{D}^4$ to each order is only added at the end of an integration step, $t_0 + \Delta t$. This semi-iteration, first introduced by von Hoerner [1960], gives increased accuracy at little extra cost (on scalar machines) and no extra memory requirement.

We now describe the initialization procedure, assuming one force polynomial. From the initial conditions, $m_j, \mathbf{r}_j, \mathbf{v}_j$, the respective Taylor series derivatives are formed by successive differentiations of (1.1). Introducing the relative coordinates, $\mathbf{R} = \mathbf{r}_i - \mathbf{r}_j$, and relative velocity, $\mathbf{V} = \mathbf{v}_i - \mathbf{v}_j$, all pair-wise interaction terms in $\mathbf{F}$ and $\mathbf{F}^{(1)}$ are first obtained by

$$\begin{aligned}
\mathbf{F}_{ij} &= -m_j\mathbf{R}/R^3 , \\
\mathbf{F}_{ij}^{(1)} &= -m_j\mathbf{V}/R^3 - 3a\mathbf{F}_{ij} ,
\end{aligned} \tag{2.4}$$

with $a = \mathbf{R} \cdot \mathbf{V}/R^2$. The total contributions are obtained by summation over all N particles. Next, the mutual second- and third-order terms are formed from

$$\begin{aligned}
\mathbf{F}_{ij}^{(2)} &= -m_j(\mathbf{F}_i - \mathbf{F}_j)/R^3 - 6a\mathbf{F}_{ij}^{(1)} - 3b\mathbf{F}_{ij} , \\
\mathbf{F}_{ij}^{(3)} &= -m_j(\mathbf{F}_i^{(1)} - \mathbf{F}_j^{(1)})/R^3 - 9a\mathbf{F}_{ij}^{(2)} - 9b\mathbf{F}_{ij}^{(1)} - 3c\mathbf{F}_{ij} ,
\end{aligned} \tag{2.5}$$

with

$$\begin{aligned}
b &= \left(\frac{V}{R}\right)^2 + \frac{\mathbf{R} \cdot (\mathbf{F}_i - \mathbf{F}_j)}{R^2} + a^2 , \\
c &= \frac{3\mathbf{V} \cdot (\mathbf{F}_i - \mathbf{F}_j)}{R^2} + \frac{\mathbf{R} \cdot (\mathbf{F}_i^{(1)} - \mathbf{F}_j^{(1)})}{R^2} + a(3b - 4a^2) .
\end{aligned} \tag{2.6}$$

A second double summation gives the corresponding values of $\mathbf{F}^{(2)}$ and $\mathbf{F}^{(3)}$ for all particles. This pair-wise *boot-strapping* procedure provides a convenient starting algorithm, since the extra cost is usually small. Here

we have employed a compact derivation [Findlay, private communication, 1983] instead of the equivalent but more cumbersome expressions used previously [cf. Aarseth, 1972b].

Appropriate initial time-steps, Δt_i, are now determined, using the general criterion discussed in the next section. Setting $t_0 = 0$, the backwards times are initialized by $t_k = -k\Delta t_i$ $(k = 1, 2, 3)$. Hence this assumes constant time-steps over the past fitting interval. Inversion of (2.3) to third order finally yields starting values for the divided differences,

$$\begin{aligned} \mathbf{D}^1 &= (\tfrac{1}{6}\mathbf{F}^{(3)}t_1' - \tfrac{1}{2}\mathbf{F}^{(2)})t_1' + \mathbf{F}^{(1)}, \\ \mathbf{D}^2 &= -\tfrac{1}{6}\mathbf{F}^{(3)}(t_1' + t_2') + \tfrac{1}{2}\mathbf{F}^{(2)}, \\ \mathbf{D}^3 &= \tfrac{1}{6}\mathbf{F}^{(3)}. \end{aligned} \tag{2.7}$$

It should be remarked that polynomial initialization may also be required at any stage of the calculation, after switching from standard integration to more sophisticated treatments and *vice versa.*

The introduction of a softened potential of the form

$$\Phi = -m/(R^2 + \epsilon^2)^{1/2} \tag{2.8}$$

is of historical interest [Aarseth, 1963a,b]. This represents a Plummer sphere [Plummer, 1911] with half-mass radius given by $r_{\rm h} \simeq 1.3\epsilon$ [Aarseth & Fall, 1980]. Originally it was used to model galaxies with ϵ representing the characteristic size, and has been employed more generally to reduce the effect of close encounters. Softening may readily be included by modifying all inverse R terms in the denominators of equations (2.4) (2.6). For some purposes, the corresponding radial force does not fall off sufficiently fast with distance and a steeper r-dependence given by $\Phi = -m/(R^4 + \epsilon^4)^{1/4}$ has been tried [Oh, Lin & Aarseth, 1995]. This representation also has the advantage that outside some distance it can be replaced by the basic point-mass interaction without significant loss of accuracy. Finally, it may be remarked that a softened potential necessitates modifying the virial expression which is often used in simulations. Neglecting external effects, the potential energy is then replaced by a double summation over $m_i\mathbf{r}_{ij} \cdot \mathbf{F}_{ij}$ which gives the virial energy

$$V = -\sum_{i=1}^{N} \sum_{j=1;\, j\neq i}^{N} \frac{m_j|\mathbf{r}_i - \mathbf{r}_j|^2}{(|\mathbf{r}_i - \mathbf{r}_j|^2 + \epsilon^2)^{3/2}}. \tag{2.9}$$

2.3 Individual time-steps

Stellar systems are characterized by a range in density that gives rise to different time-scales for significant changes of the orbital parameters.

In order to exploit this feature, and economize on the expensive force calculation, each particle is assigned its own time-step which is related to the orbital time-scale. Thus the aim is to ensure convergence of the force polynomial (2.1) with the minimum number of force evaluations. Since all interactions must be added consistently in a direct integration method, it is necessary to include a temporary coordinate prediction of the other particles. However, the additional cost of low-order predictions still leads to a significant overall saving since this permits a wide range of time-steps to be used.

Following the polynomial initialization discussed above, the integration cycle itself begins by determining the next particle, i, to be advanced; i.e. the particle, j, with the smallest value of $t_j + \Delta t_j$, where t_j is the time of the last force evaluation. It is convenient to define the present epoch, or 'global' time, t, at this endpoint, rather than adding a small interval to the previous value. The complete integration cycle consists of the sequence given by Algorithm 2.1.

Algorithm 2.1. *Individual time-step cycle.*

1	Determine the next particle: $i = \min_j \{t_j + \Delta t_j\}$
2	Set the new global time by $t = t_i + \Delta t_i$
3	Predict all coordinates $\mathbf{r}_j$ to order $\mathbf{F}^{(1)}$
4	Form $\mathbf{F}^{(2)}$ by the second equation (2.3)
5	Improve $\mathbf{r}_i$ and predict $\mathbf{v}_i$ to order $\mathbf{F}^{(3)}$
6	Obtain the new force $\mathbf{F}_i$
7	Update the times t_k and differences $\mathbf{D}^k$
8	Apply the corrector $\mathbf{D}^4$ to $\mathbf{r}_i$ and $\mathbf{v}_i$
9	Specify the new time-step Δt_i
10	Repeat the calculation at step 1

The individual time-step scheme [Aarseth, 1963a,b] uses two types of coordinates for each particle. We define primary and secondary coordinates, $\mathbf{r}_0$ and $\mathbf{r}_t$, evaluated at t_0 and t, respectively, where the latter are derived from the former by the predictor. In the present treatment, unless high precision is required, we predict all the coordinates to order $\mathbf{F}^{(1)}$ by

$$\mathbf{r}_j = [(\tfrac{1}{6}\mathbf{F}^{(1)}\delta t_j' + \tfrac{1}{2}\mathbf{F})\delta t_j' + \mathbf{v}_0]\delta t_j' + \mathbf{r}_0\,, \tag{2.10}$$

where $\delta t_j' = t - t_j$ (with $\delta t_j' \leq \Delta t_j$). The coordinates and velocity of particle i are then improved to order $\mathbf{F}^{(3)}$ by standard Taylor series integration (cf. 2.3), whereupon the current force is calculated by direct summation. At this stage the four times t_k are updated (i.e. replacing t_k with t_{k-1}) to be consistent with the definition that t_0 denotes the time

of the most recent force evaluation. New differences are now formed (cf. 2.2), including $\mathbf{D}^4$. Together with the new $\mathbf{F}^{(4)}$, these correction terms are combined to improve the current coordinates and velocity to highest order. The coordinate and velocity increments of (2.1) due to the corrector $\mathbf{D}^4$ contain four terms since all the lower derivatives are also modified in (2.3). Consequently, we combine the corresponding time-step factors which yield in compact notation, with $t' = t - t_0$

$$\begin{aligned} \Delta\mathbf{r}_i &= \mathbf{F}^{(4)} \left\{ [(\tfrac{2}{3}t' + c)0.6t' + b]\tfrac{1}{12}t' + \tfrac{1}{6}a \right\} t'^3 , \\ \Delta\mathbf{v}_i &= \mathbf{F}^{(4)} \left\{ [(0.2t' + 0.25c)t' + \tfrac{1}{3}b]t' + 0.5a \right\} t'^2 , \end{aligned} \tag{2.11}$$

where all factorials are absorbed in the force derivatives. The coefficients are defined by $a = t_1' t_2' t_3'$, $b = t_1' t_2' + t_1' t_3' + t_2' t_3'$, $c = t_1' + t_2' + t_3'$, respectively, where the old definition of t_k' still applies. Finally, the primary coordinates are initialized by setting $\mathbf{r}_0 = \mathbf{r}_t$. Hence we have a fourth-order predictor–corrector scheme.

New time-steps are assigned initially for all particles and at the end of each integration cycle for particle i. General considerations of convergence for the corresponding Taylor series (2.1) suggest a time-step of the type

$$\Delta t_i = \left(\frac{\eta |\mathbf{F}|}{|\mathbf{F}^{(2)}|} \right)^{1/2} , \tag{2.12}$$

where η is a dimensionless accuracy parameter. Such an expression would have the desirable property of ensuring similar *relative* errors of the force. Moreover, two particles of different mass interacting strongly would tend to have very similar time-steps, which also has certain practical advantages. However, there are situations when this simple form is less satisfactory. After considerable experimentation, we have adopted a more sensitive composite criterion given by

$$\Delta t_i = \left(\frac{\eta(|\mathbf{F}||\mathbf{F}^{(2)}| + |\mathbf{F}^{(1)}|^2)}{|\mathbf{F}^{(1)}||\mathbf{F}^{(3)}| + |\mathbf{F}^{(2)}|^2} \right)^{1/2} . \tag{2.13}$$

For this purpose only the last two terms of the first and second force derivatives in (2.3) are included. This expression ensures that all the force derivatives play a role and it is also well defined for special cases (i.e. starting from rest or $|\mathbf{F}| \simeq 0$). Although successive time-steps normally change smoothly, it is prudent to restrict the growth by an inertial factor (e.g. 1.2). Being more sensitive, typical time-steps are about $\sqrt{2}$ times smaller than given by (2.12) for the same value of η.

In summary, the scheme requires the following 30 variables for each particle: m, $\mathbf{r}_0$, $\mathbf{r}_t$, $\mathbf{v}_0$, $\mathbf{F}$, $\mathbf{F}^{(1)}$, $\mathbf{D}^1$, $\mathbf{D}^2$, $\mathbf{D}^3$, Δt, t_0, t_1, t_2, t_3. It is also useful to employ a secondary velocity, denoted $\mathbf{v}_t$, for dual purposes, such as temporary predictions and general evaluations.