Algorithms to solve Newton's Laws on a Computer

1 The Euler Algorithm

Newtons' Second Law of motion relates the second derivatives of the position coordinates of a particle to its acceleration components, which are, in general, functions of its position, velocity and time. Consider a particle in one dimension, with position coordinate x measured with respect to a suitable origin. Newton's Second Law for this particle then reduces to the general form

$$\frac{d^2x}{dt^2} = a(x,v,t) \tag{1}$$

where $v = dx/dt$ is the velocity of the particle. This second order differential equation can be written as a pair of coupled first order differential equations in the position $x(t)$ and velocity $v(t)$ of the particle

$$\begin{aligned} \frac{dx}{dt} &= v \\ \frac{dv}{dt} &= a(x,v,t) \end{aligned} \tag{2}$$

Given the position $x(t_0)$ and velocity $v(t_0)$ at some instant t_0, the position and velocity at any other instant of time are uniquely determined. There are many algorithms that can be implemented on a computer to compute $x(t_f)$ and $v(t_f)$ at instant t_f. These rely on 'slicing' the finite time interval $t_f - t_0$ into N 'small' intervals of size $\Delta t = (t_f - t_0)/N$, such that given $x(t)$ and $v(t)$ at any intermediate instant between t_0 and t_f, $x(t+\Delta t)$ and $v(t+\Delta t)$ can be determined to some predefined accuracy. Such algorithms then allow one to 'hop' from one instant to another, starting at t_0 and ending at t_f. These algorithms rely on the Taylor expansion of a function f of t about a point t

$$f(t+\Delta t) = f(t) + \Delta t\ \dot{f}(t) + \frac{\Delta t^2}{2!}\ \ddot{f}(t) + \frac{\Delta t^3}{3!}\ \dddot{f}(t) + \frac{\Delta t^4}{4!}\ \ddddot{f}(t) + ... \tag{3}$$

where $\dot{f} = df/dt$, $\ddot{f} = d^2f/dt^2$, $\dddot{f} = d^3f/dt^3$, etc. Any given algorithm involves the effective truncation of this series after a finite number of terms, introducing an error of a given order. The Euler algorithm involves truncating the series after the term of order Δt, introducing an error of order Δt^2 or higher

$$f(t+\Delta t) = f(t) + \Delta t\ \dot{f}(t) + \mathcal{O}(\Delta t^2) \tag{4}$$

Applied to the position coordinate $x(t)$ and velocity $v(t)$, this algorithm gives

$$\begin{aligned} x(t+\Delta t) &= x(t) + \Delta t\ \dot{x}(t) + \mathcal{O}(\Delta t^2) \\ &= x(t) + \Delta t\ v(t) + \mathcal{O}(\Delta t^2) \\ v(t+\Delta t) &= v(t) + \Delta t\ \dot{v}(t) + \mathcal{O}(\Delta t^2) \\ &= v(t) + \Delta t\ a(t) + \mathcal{O}(\Delta t^2) \end{aligned} \tag{5}$$

Since the Second Law gives the acceleration at instant t as a function of position and velocity at that instant, therefore, the Euler Algorithm reduces to

$$\boxed{\begin{aligned} x(t+\Delta t) &= x(t) + \Delta t\ v(t) \\ v(t+\Delta t) &= v(t) + \Delta t\ a\left[x(t), v(t), t\right] \end{aligned}}$$

Clearly, given $x(t)$ and $v(t)$, this algorithm allows us to determine $x(t+\Delta t)$ and $v(t+\Delta t)$ up to accuracy of order Δt in each 'hop', introducing an error of order Δt^2. However, after N such steps, the cumulative error is of order $N\Delta t^2$ which is of order $(t_f - t_0)\Delta t$. Clearly, this error need not be small for a large enough time interval $(t_f - t_i)$.

2 The Verlet Algorithm

If the acceleration of the particle is only a function of its position, the Verlet Algorithm is an improvement over the Euler Algorithm. Apart from being accurate up to order Δt^2 (that is, the error in each step is order Δt^3 or higher), it has some special mathematical properties [1], which make it especially suitable when systems are to be evolved for long durations of time. The Verlet Algorithm is a three-step algorithm, unlike the Euler Algorithm, which is a two-step algorithm. Given the position and velocity at instant t, it computes these at $t+\Delta t$ at a higher accuracy (relative to the Euler Algorithm) by involving the values of x and v at the intermediate instant $t+\Delta t/2$

$$\boxed{\begin{aligned} x(t+\Delta t/2) &= x(t) + \frac{\Delta t}{2} v(t) \\ v(t+\Delta t) &= v(t) + \Delta t\ a(t+\Delta t/2) \\ x(t+\Delta t) &= x(t+\Delta t/2) + \frac{\Delta t}{2} v(t+\Delta t) \end{aligned}}$$

In the second step, the acceleration at instant $t+\Delta t/2$ is computed by using the value of the position at this instant (since the acceleration is a function of position only). A key idea used in this algorithm is that given a function at some instant t, its value at instant $t+\Delta t$ is known to accuracy Δt^2, if its derivative is known at the half-step $t+\Delta t/2$

$$f(t+\Delta t) = f(t) + \Delta t\ \dot{f}(t+\Delta t/2) + \mathcal{O}(\Delta t^3) \tag{6}$$

This claim can be proved by expanding $\dot{f}(t+\Delta t/2)$ in a Taylor series about t and retaining terms up to order Δt only

$$\dot{f}(t+\Delta t/2) = \dot{f}(t) + \frac{\Delta t}{2}\ddot{f}(t) + \mathcal{O}(\Delta t^2) \tag{7}$$

Substituting this in eqn.(6), we see that since we have Δt as a coefficient of $\dot{f}(t+\Delta t/2)$, the $\mathcal{O}(\Delta t^2)$ error will result in an effective $\mathcal{O}(\Delta t^3)$ error

$$\begin{aligned} f(t+\Delta t) &= f(t) + \Delta t\left[\dot{f}(t) + \frac{\Delta t}{2}\ddot{f}(t) + \mathcal{O}(\Delta t^2)\right] && (8) \\ &= f(t) + \Delta t\ \dot{f}(t) + \frac{\Delta t^2}{2}\ \ddot{f}(t) + \mathcal{O}(\Delta t^3) && (9) \end{aligned}$$

which we identify as the standard Taylor expansion accurate up to order Δt^2. Given this, we notice that in the three-step Verlet Algorithm, the second step is accurate, by itself, up to order Δt^2 (since $a(t) = \dot{v}(t)$). Further, taken *together*, the first and third step are accurate up to order Δt^2. To see this, we substitute the first step in the third, to get

$$\begin{aligned} x(t+\Delta t) &= x(t+\Delta t/2) + \frac{\Delta t}{2}\ v(t+\Delta t) \\ &= x(t) + \frac{\Delta t}{2}\ v(t) + \frac{\Delta t}{2}\ v(t+\Delta t) && (10) \end{aligned}$$

[1] It is symplectic, preserving phase space volumes. As a result, trajectories are bounded.

Expanding $v(t+\Delta t)$ in a Taylor series, we get

$$\begin{aligned} x(t+\Delta t) &= x(t) + \frac{\Delta t}{2}\ v(t) + \frac{\Delta t}{2}\left[v(t) + \Delta t\ a(t) + \mathcal{O}(\Delta t^2)\right] \\ &= x(t) + \frac{\Delta t}{2}\ v(t) + \frac{\Delta t}{2}\ v(t) + \frac{\Delta t^2}{2}\ a(t) + \mathcal{O}(\Delta t^3) \\ &= x(t) + \Delta t\ v(t) + \frac{\Delta t^2}{2}\ a(t) + \mathcal{O}(\Delta t^3) \end{aligned} \tag{11}$$

which is the Taylor expansion for $x(t+\Delta t)$ correct up to order Δt^2.

3 The Second Order Runge Kutta Algorithm

The Second Order Runge Kutta (RK) Algorithm is a powerful algorithm that computes position and velocity up to order Δt^2 accuracy, for arbitrary acceleration functions. It relies on computing a function by using information about its derivative at a half-step, as in equation (6). Let us start by computing the position at instant $t+\Delta t$

$$x(t+\Delta t) = x(t) + \Delta t\ v(t+\Delta t/2) + \mathcal{O}(\Delta t^3) \tag{12}$$

In the above equation, we can expand $v(t+\Delta t/2)$ in a Taylor series up to order Δt, leaving an over all error of order Δt^3, since $v(t+\Delta t/2)$ comes with Δt as coefficient

$$v(t+\Delta t/2) = v(t) + \frac{\Delta t}{2} a(t) \tag{13}$$

Since we know the acceleration as a function of position, velocity and time, given the position and velocity at time t allows us to compute $v(t+\Delta t/2)$ in the above equation, which we then use in the equation for $x(t+\Delta t)$. Then, the position at $t+\Delta t$ is determined as follows

$$x(t+\Delta t) = x(t) + \Delta t\left[v(t) + \frac{\Delta t}{2} a\left[x(t), v(t), t\right]\right] \tag{14}$$

Next, we compute the velocity at $t+\Delta t$

$$v(t+\Delta t) = v(t) + \Delta t\ a(t+\Delta t/2) + \mathcal{O}(\Delta t^3) \tag{15}$$

Now,

$$a(t+\Delta t/2) = a\left[x(t+\Delta t/2), v(t+\Delta t/2), t+\Delta t/2\right] \tag{16}$$

To compute the acceleration at $t+\Delta t/2$, we can expand $x(t+\Delta t/2)$ and $v(t+\Delta t/2)$ (on which $a(t+\Delta t/2)$ depends on) up to order Δt, since this will result in an effective error of order Δt^3 (since $a(t+\Delta t/2)$ has Δt as coefficient). Then, we use

$$\begin{aligned} x(t+\Delta t/2) &= x(t) + \frac{\Delta t}{2}\ v(t) \\ v(t+\Delta t/2) &= v(t) + \frac{\Delta t}{2}\ a(t) \\ &= v(t) + \frac{\Delta t}{2}\ a\left[x(t), v(t), t\right] \end{aligned} \tag{17}$$

Therefore, the velocity at $t+\Delta t$ is determined as follows

$$v(t+\Delta t) = v(t) + \Delta t\ a\left[x(t) + \frac{\Delta t}{2}\ v(t), v(t) + \frac{\Delta t}{2}\ a\left[x(t), v(t), t\right], t+\Delta t/2\right] \tag{18}$$

In a nutshell, the algorithm is

$$\boxed{\begin{aligned} x(t+\Delta t) &= x(t) + \Delta t \left[v(t) + \frac{\Delta t}{2} a\left[x(t), v(t), t\right] \right] \\ v(t+\Delta t) &= v(t) + \Delta t \ a \left[x(t) + \frac{\Delta t}{2} \ v(t), v(t) + \frac{\Delta t}{2} \ a\left[x(t), v(t), t\right], t + \Delta t/2 \right] \end{aligned}}$$