The numerical solution of Newton's equations relies on breaking up the motion into small time steps, δt. For example, if you know $x(t=0)$ and $v(t=0)$, you can get them at $t = 5s$ by first finding $x(t=0.01s)$, $v(t=0.01s)$, then at $0.02s$, and so on.

The solution will always be <u>approximate</u>.

Tools to find a prescription that takes $x(t_1), v(t_1)$ to $x(t_2), v(t_2)$ include calculus and the Taylor series expansion.

Solving Newton's equation by stepping in time

Direct use of 2^{nd} deriv

$$\ddot{x}(t) = \underbrace{F}_{\text{force}}(\overbrace{x(t)}^{\text{position}}, t)/\underbrace{m}_{\text{mass}} = \underbrace{a}_{\text{acceleration}}(x(t), t)$$

① Use the Taylor series expansion to show

$$\frac{x(\delta t) - 2x(0) + x(-\delta t)}{\delta t^2} = \ddot{x}(0) + O(\delta t^2)$$

② Use Taylor series to show $\dfrac{x(t+\delta t) - 2x(t) + x(t-\delta t)}{\delta t^2} = \ddot{x}(t) + O(\delta t^2)$

Algorithm 1

Use Newton's equation to get an expression for $\ddot{x}(t)$

③ Show $x(t+\delta t) = 2x(t) - x(t-\delta t) + \delta t^2\, a(x(t),t) + O(\delta t^4)$

Algorith: start with $x(0)$ and $x(-\delta t)$
use $x(0)$ to compute $a(x(0), 0)$
compute $x(\delta t) = 2x(0) - x(-\delta t) + \delta t^2\, a(x(0), 0)$
use $x(\delta t)$ to compute $a(x(\delta t), \delta t)$
compute $x(2\delta t) = 2x(\delta t) - x(0) + \delta t^2\, a(x(\delta t), \delta t)$
⋮

Advantage – high order accuracy for little work
Disadvantage – some forces depend on $v(t)$, fixed time step
need $x(0)$, $x(-\delta t)$ but usually have $x(0)$, $v(0)$

Use 2 1st Deriv

④ Show Newton's equation is the same as
$\dot{X}_1(t) = X_2(t)$ and $\dot{X}_2(t) = a(X_1(t), t)$
where $X_1(t) \equiv X(t)$ and $X_2(t) \equiv V(t)$

⑤ Show $\frac{f(\delta t) - f(0)}{\delta t} = \dot{f}(0) + O(\delta t)$

⑥ Show $\frac{f(t+\delta t) - f(t)}{\delta t} = \dot{f}(t) + O(\delta t)$

Euler's method

This approximation can be used to find a new algorithm

$$X_1(t+\delta t) = X_1(t) + X_2(t)\,\delta t + O(\delta t^2)$$
$$X_2(t+\delta t) = X_2(t) + a(X_1(t), t)\,\delta t + O(\delta t^2)$$

Algorithm: start with $X_1(0) = X(0)$ and $X_2(0) = V(0)$
use $X_1(0)$ to compute $a(X_1(0), 0)$
Compute $X_1(\delta t) = X_1(0) + X_2(0)\,\delta t$
$X_2(\delta t) = X_2(0) + a(X_1(0), 0)\,\delta t$
use $X_1(\delta t)$ to compute $a(X_1(\delta t), \delta t)$
compute $X_1(2\delta t) = X_1(\delta t) + X_2(\delta t)\,\delta t$
$X_2(2\delta t) = X_2(\delta t) + a(X_1(\delta t), \delta t)\,\delta t$
⋮

Advantage - will work if a also depends on V
starts with $X(0), V(0)$; only uses 1st derivative
Disadvantages - low order method, energy will drift

You want to compute $X(t_f), V(t_f)$ [t_f is the final time] given an initial t_0.

⑦ Show that the accuracy is proportional to $1/N$ where N is the number of time steps. (Hint: how does the accuracy of 1 time step depend on N.)

2^{nd} Order Runge-Kutta

A method with higher order accuracy uses two calculations per time step.

Suppose you have $\dot{X} = F(X(t), t)$

(1) Show that the following sequence has the stated accuracy

$$\bar{X} \equiv X(t) + \frac{\delta t}{2} F(X(t), t)$$
$$X(t+\delta t) = X(t) + \delta t \cdot F\left(\bar{X}, t+\frac{\delta t}{2}\right) + \underline{\underline{O(\delta t^3)}}$$

Algorithm: start $X_1(0) = X(0)$ and $X_2(0) = V(0)$

use $X_1(0)$ to compute $a(X_1(0), 0)$

compute $X_{1temp} = X_1(0) + \frac{\delta t}{2} X_2(0)$

$X_{2temp} = X_2(0) + \frac{\delta t}{2} a(X_1(0), 0)$

use X_{1temp} to compute $a(X_{1temp}, \delta t/2)$

compute $X_1(\delta t) = X_1(0) + \delta t \cdot X_{2temp}$

$X_2(\delta t) = X_2(0) + \delta t \cdot a(X_{1temp}, \delta t/2)$

⋮

(2) Show that the accuracy of $X(t_f), V(t_f)$ is proportional to $1/N^2$ where N is the number of time steps.