PH621: Computational methods for physicists

Ref: 1) Numerical methods for Engineers
- Steven Chapra & R.P. Canale

2) Elementary numerical analysis
- Conte & Boor

Mathematical modeling of a physical process

Formulation of certain mathematical equation that can capture the essence of a physical process.

- Particle moving in a gravitational / EM field
- Heat flow
- Two particle colliding etc.

What are the types of equations for the physical process?

- Simple algebraic equation
- Differential / integral or it can be integro - differential eqn. etc

Models are formed by observation and experiment.

- Based on observation Newton formulated his laws

  His second law

  $$\vec{F} = m\vec{a}$$

- Reproducible results are obtained
- Now note that this is a simplification of reality:

  Relativistic effects & quantum features are ignored.

Example of mathematical modeling:

Parachutist problem

How do we model this process?

Can we predict the velocity of parachutist at various instants of time?

What are the forces acting on the body?

- Gravitational force pulling him down (F_D)
- Upward force due to air resistance (F_U)

Net force acting the system are:

$$\boxed{\vec{F}_{net} = \vec{F}_D + \vec{F}_U}$$

$$\vec{F}_D = mg \downarrow$$

$$\vec{F}_U = -cv \uparrow$$

m : mass of body

g : acceleration due to gravity

c : Drag coeff.

v : Velocity of body

$$\vec{F}_{net} = \vec{F}_D + \vec{F}_v$$

$$F_{net} = mg - cv$$

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$$ma = mg - cv$$

$$m\frac{dv}{dt} = mg - cv$$

$$\frac{dv(t)}{dt} = g - \frac{c}{m}v(t)$$

By solving we get $v(t)$

$$\frac{dv(t)}{dt} = g - \frac{c}{m} v(t)$$

$$= f(t)$$

$$\frac{df}{dt} = -\frac{c}{m} \frac{dv}{dt}$$

$$\frac{df}{dt} = -\frac{c}{m} f(t)$$

$$f(t) = e^{-\frac{c}{m}t} A$$

$t = 0 \qquad v(t=0) = 0$ Given initial condition

$$\Rightarrow y(t=0) = g$$

$$\Rightarrow \quad f(t) = g\, e^{-\frac{c}{m}t}$$

$$g - \frac{c}{m} v(t) = g\, e^{-\frac{c}{m}t}$$

$$\therefore \frac{c}{m} v(t) = g\left(1 - e^{-\frac{c}{m}t}\right)$$

$$v(t) = \frac{mg}{c}\left[1 - e^{-\frac{c}{m}t}\right]$$

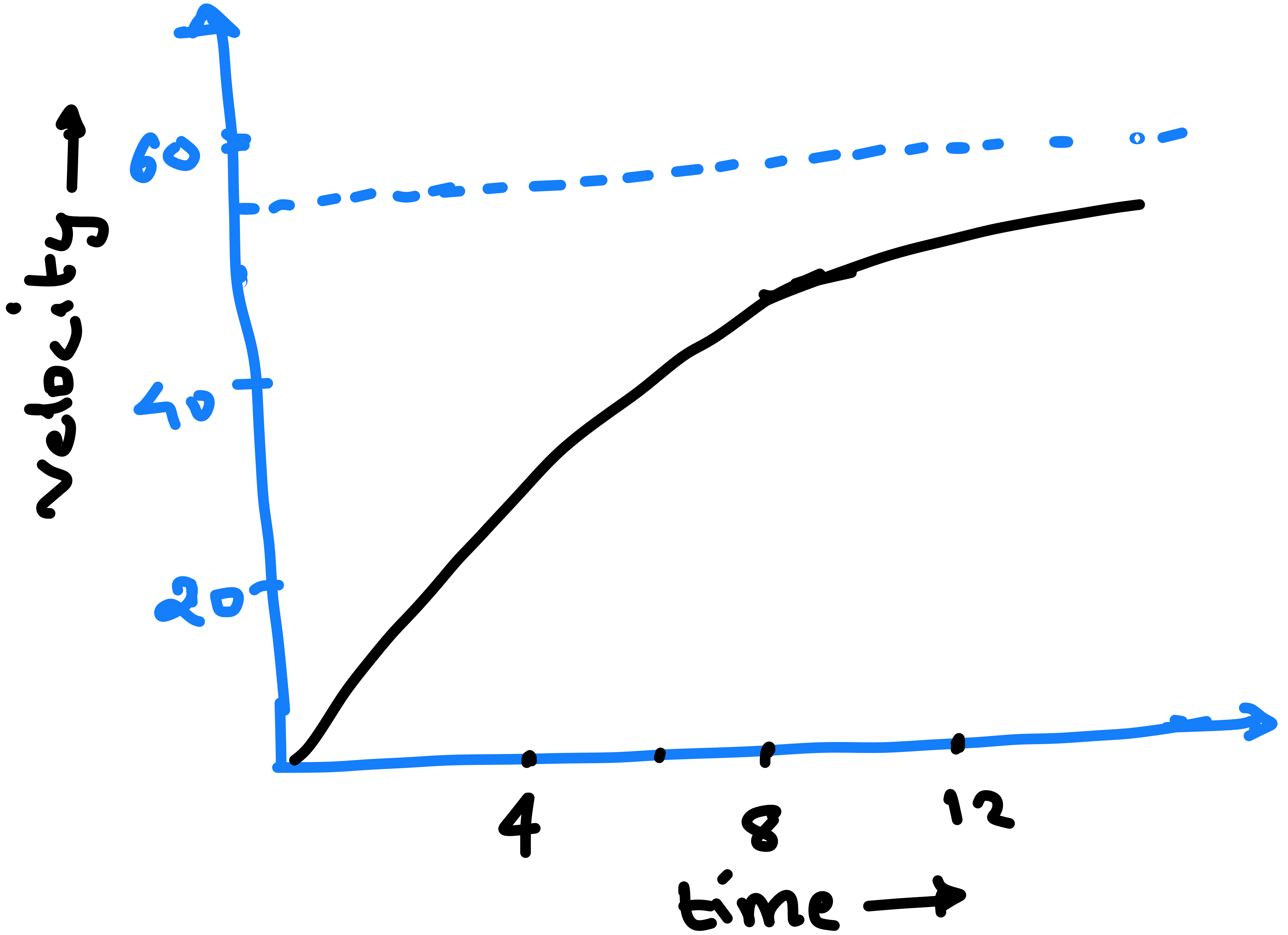
- Here we have an analytical solun.
- Using the above eqn., we can predict velocity of the body at various instants if we are given the constants in the problem (m, g, c).

$m = 68.1\ kg$, $c = 12.5\ kg/s$, $g = 9.8\ m/s^2$

$$\boxed{v(t) = \frac{mg}{c}\left[1 - e^{-\frac{c}{m}t}\right]}$$

t	v
0	0.00
2	16.40
4	27.77
6	35.64
⋮	⋮
∞	53.39

Terminal velocity



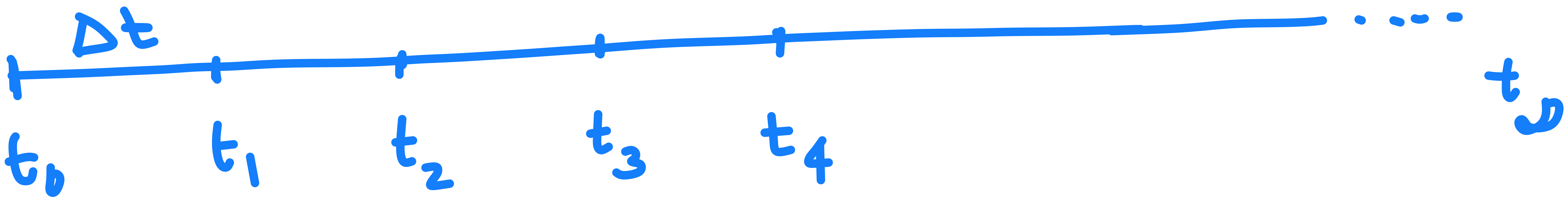
Now letz do this problem numerically:

$$\frac{dv}{dt} = \left[g - \frac{c}{m} v\right] \approx \frac{\Delta v}{\Delta t}$$

$$\frac{\Delta v}{\Delta t} = \frac{v(t+\Delta t) - v(t)}{t+\Delta t - t}$$

$t+\Delta t \rightarrow t_{i+1}$

$t \rightarrow t_i$



$t+\Delta t \rightarrow t_{i+1}$

$t \rightarrow t_i$

$$\frac{\Delta v}{\Delta t} = \frac{v(t+\Delta t) - v(t)}{t+\Delta t - t}$$

$$\left[\frac{\Delta v}{\Delta t}\right]_{t=t_i} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

$$\frac{v(t_{i+1}) - v(t_i)}{\Delta t} = \left[g - \frac{c}{m} v(t_i)\right]$$

$$\frac{v(t_{i+1}) - v(t_i)}{\Delta t} = \left[g - \frac{c}{m} v(t_i)\right]$$

$$v(t_{i+1}) - v(t_i) = \left[g - \frac{c}{m} v(t_i)\right] \Delta t$$

$$v(t_{i+1}) = v(t_i) + \left[g - \frac{c}{m} v(t_i)\right] \Delta t$$

Given velocity at i^{th} instant of time, velocity at $(i+1)^{th}$ instant can be calculated.

$$\frac{dv}{dt} = \left[g - \frac{c}{m} v(t)\right] \longrightarrow v(t_{i+1}) = v(t_i) + \left[g - \frac{c}{m} v(t_i)\right] \Delta t$$

diff. eqn $\longrightarrow$ Simple arithmetic operations

Basically, we have re-written the differential eqn. in such a way that, 'v' at any instant of time can be calculated by using simple arithmetic operations

$$v(t_{i+1}) = v(t_i) + \left[g - \frac{c}{m} v(t_i)\right] \Delta t$$

Now letz calculate $v(t_{i+1})$

→ Start with $i = 0$, $\Delta t = 2$

$$v(t_1) = v(t_0) + \left[g - \frac{c}{m} v(t_0)\right] \times 2$$

$$v(t_0) = 0$$

$$\therefore \quad v(t_1) = 2g = 19.6 \text{ m/s}$$

Using $v(t_1)$, we can calculate $v(t_2)$

→ $v(t_2) = ?$ (i.e. velocity at 4th sec)

$$v(t_2) = v(t_1) + \left[g - \frac{c}{m} v(t_1) \right] \Delta t$$

$$= 19.6 + \left(9.8 - \frac{12.5}{68.1} \times 19.6 \right) 2$$

$$= 32.00 \text{ m/s}$$

→ $v(t_3) = ?$ ($t_3 = 6$ sec)

$$v(t_3) = v(t_2) + \left[g - \frac{c}{m} v(t_2) \right] \Delta t$$

$$= 39.85 \text{ m/s}$$

Analytical solu^n.

t	v
0	0.00
2	16.40
4	27.77
6	35.64
⋮	⋮
∞	53.39

Numerical solun.

t	v
0	0
2	19.6
4	32.00
6	39.86
⋮	⋮
∞	53.39

Although our numerical solun. showing the same trend, but there are differences in values at each instants.

Now instead of using $\Delta t = 2$ sec, letz use $\Delta t = 1$ sec

$$\rightarrow v(t_1) = v(t_0) + \left[g - \frac{c}{m} v(t_0)\right] \times 1 \qquad v(t_0) = 0$$

$$= 9.8 \text{ m/s}$$

$\rightarrow v(t_2)$ [i.e. $t = 2$ sec]

$$v(t_2) = v(t_1) + \left[g - \frac{c}{m} v(t_1)\right] \times 1$$

$$= 9.8 + \left[9.8 - \frac{12.5}{68.1} \times 9.8\right]$$

$$= 17.8 \text{ m/s}$$

Analytical

t	v
0	0.00
2	16.40
4	27.77
6	35.64
⋮	⋮
∞	53.39

Numerical

$\Delta t = 2$

t	v
0	0
2	19.6
4	32.00
6	39.86
⋮	⋮
∞	53.39

Numerical

$\Delta t = 1$

t	v
0	0
1	9.8
2	17.8
⋮	⋮
∞	53.39

$\Delta t = 0.5$

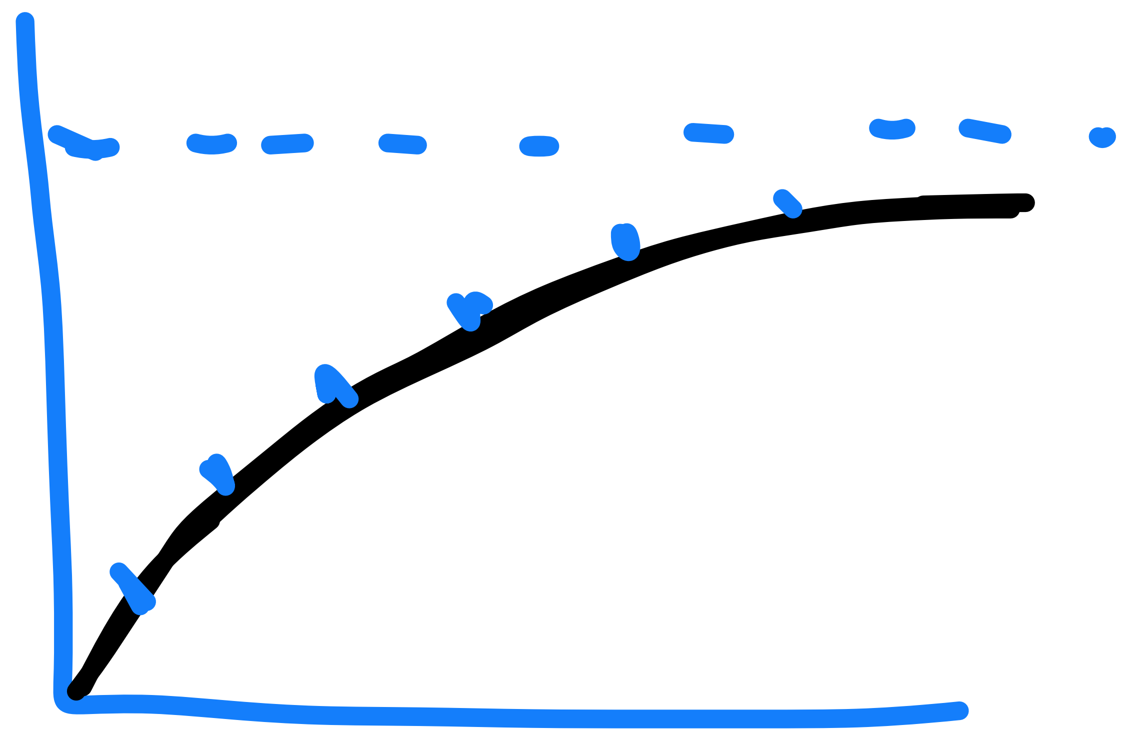
0	
0.5	
1.0	
1.5	
2	17.06

As the Δt (step-size) decreases, we are getting better results

Our arithmetic operation actually corresponding to a straight-line approximation

$$V(t_{i+1}) = V(t_i) + \left[g - \frac{c}{m} v\right] \Delta t$$

$$V_{NEW} = V_{old} + (\text{slope}) \times \Delta t$$



if we take points closer and closer, straight line approximation works better

Just to summarize:

$$\frac{dv}{dt} = \left[g - \frac{c}{m} v(t)\right]$$

$$\frac{dv}{dt} \approx \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

[Finite divided difference approximation]

Using this approx^n.

$$v(t_{i+1}) = v(t_i) + \left[g - \frac{c}{m} v(t_i)\right] \times \Delta t$$

$$\boxed{V_{NEW} = V_{old} + (\text{slope}) \times (\text{step-size})}$$

[Euler's method]