### Chapter 9

Solving Second order differential equations numerically, 2

#### Online lecture materials

- •The online lecture notes by Dr. Tai-Ran Hsu of San José State University,
- http://www.engr.sjsu.edu/trhsu/Chapt er%204%20Second%20order%20DEs.p df

provides a very clear explanation of the solutions and applications of some typical second order differential equations.

#### 2<sup>nd</sup> Order Homogeneous DEs

$$\frac{d^2u(x)}{dx^2} + a\frac{du(x)}{dx} + bu(x) = 0$$

with <u>TWO</u> given conditions The solutions

Case 1: 
$$a^2 - 4b > 0$$
:  
$$u(x) = e^{-\frac{ax}{2}} \left( c_1 e^{\sqrt{a^2 - 4b} x/2} + c_2 e^{-\sqrt{a^2 - 4b} x/2} \right)$$

<u>Case 2:  $a^2 - 4b < 0$ </u>:

$$u(x) = e^{-\frac{ax}{2}} \left[ A \operatorname{Sin}\left(\frac{1}{2}\sqrt{4b-a^2}\right) x + B \operatorname{Cos}\left(\frac{1}{2}\sqrt{4b-a^2}\right) x \right]$$

<u>Case 3:  $a^2 - 4b = 0$ </u>: — A special case

$$u(x) = c_1 e^{-\frac{ax}{2}} + c_2 x e^{-\frac{ax}{2}} = (c_1 + c_2 x) e^{-\frac{ax}{2}}$$
(4.12)

where c<sub>1</sub>, c<sub>2</sub>, A and B are arbitrary constants to be determined by given conditions

**Example 4.1** Solve the following differential equation

$$\frac{d^{2}u(x)}{dx^{2}} + 5\frac{du(x)}{dx} + 6u(x) = 0$$

$$u(x) = e^{-5x/2} \left( c_1 e^{x/2} + c_2 e^{-x/2} \right) = c_1 e^{-2x} + c_2 e^{-3x}$$

where c<sub>1</sub> and c<sub>2</sub> are arbitrary constants to be determined by given conditions

#### Example 4.2

$$\frac{d^2u(x)}{dx^2} + 6\frac{du(x)}{dx} + 9u(x) = 0$$

$$\frac{u(0) = 2}{\frac{du(x)}{dx}}\Big|_{x=0} = 0$$

$$u(x) = 2(1+3x)e^{-3x}$$

### DSolve

•DSolve of Mathematica can provide analytical solution to a generic second order differential equation. See Math built in 20DE.nb.

### Typical second order, non-homogeneous ordinary differential equations

$$\frac{d^{2}u(x)}{dx^{2}} + a\frac{du(x)}{dx} + bu(x) = n(x)$$
(4.25)
Non-homogeneous term

Solution of Equation (4.25) consists **TWO** components:

Solution u(x) = 
$$\begin{array}{c} Complementary \\ solution u_h(x) \end{array}$$
 +  $\begin{array}{c} Particular \\ solution u_p(x) \end{array}$ 

 $u(x) = u_h(x) + u_p(x)$ 

### Typical second order, non-homogeneous ordinary differential equations

$$\frac{d^{2}u(x)}{dx^{2}} + a\frac{du(x)}{dx} + bu(x) = n(x)$$
(4.25)
Non-homogeneous term

$$u(x) = u_h(x) + u_p(x)$$
$$\frac{d^2 u_h(x)}{dx^2} + a \frac{d u_h(x)}{dx} + b u_h(x) = 0$$

There is **NO** fixed rule for deriving  $u_p(x)$ 

#### Example 4.6

$$\frac{d^2 y(x)}{dx^2} - \frac{dy(x)}{dx} - 2y(x) = \sin 2x$$

 $y(x) = y_h(x) + y_p(x)$ 

$$\frac{d^2 y_h(x)}{dx^2} - \frac{dy_h(x)}{dx} - 2y_h(x) = 0$$
  
$$y_h(x) = c_1 e^{-x} + c_2 e^{2x}$$

Guess:  $y_p(x) = A \operatorname{Sin} 2x + B \operatorname{Cos} 2x$ After some algebra  $y(x) = y_h(x) + y_p(x) = c_1 e^{-x} + c_2 e^{2x} + \left(-\frac{3}{20} \operatorname{Sin} 2x + \frac{1}{20} \operatorname{Cos} 2x\right)$ 

#### Example 4.8

$$\frac{d^2u(x)}{dx^2} + 4u(x) = 2Sin2x$$

$$u(x) = u_h(x) + u_p(x) = c_1 \cos 2x + c_2 \sin 2x - \frac{x}{2} \cos 2x$$

. .

#### Simple Harmonic pendulum as a special case of second order DE

Force on the pendulum  $F_{\theta} = -m g \sin \theta$ 

for small oscillation,  $\sin\theta \approx \theta$ .

Equation of motion (EoM)

dx

$$F_{\theta} = ma_{\theta}$$

$$mgsin\theta = m\frac{dv_{\theta}}{dt} = m\frac{d}{dt}\left(\frac{dr}{dt}\right) \approx m\frac{d^{2}}{dt^{2}}(l\theta)$$

$$\frac{d^{2}\theta}{dt^{2}} \approx -\frac{g\theta}{l}$$

$$\frac{^{2}u(x)}{dx^{2}} + a\frac{du(x)}{dx} + bu(x) = n(x)$$

$$F_{\theta}$$
The period of the SHO is given by
$$T = 2\pi\sqrt{\frac{l}{dt}}$$



A

Simple Harmonic pendulum as a special case of second order DE (cont.)

$$\frac{d^{2}u(x)}{dx^{2}} + a\frac{du(x)}{dx} + bu(x) = n(x)$$

$$x \equiv t$$

$$u(x) \equiv \theta(t)$$

$$a \equiv 0$$

$$b \equiv \frac{g}{l}$$

$$n(x) \equiv 0$$

$$\frac{d^{2}\theta(t)}{dt^{2}} = -\frac{g\theta}{l}$$

Simple Harmonic pendulum as a special case of second order DE (cont.)

$$\frac{d^2\theta(t)}{dt^2} = -\frac{g\theta}{l}$$

Analytical solution:

 $\theta = \theta_0 \sin(\Omega t + \phi)$ 

 $\Omega = \sqrt{g/l}$  natural frequency of the pendulum;  $\theta_0$  and  $\phi$  are constant determined by boundary conditions

## Simple Harmonic pendulum with drag force as a special case of second order DE

Drag force on a moving object,  $f_d = -kv$ 

For a pendulum, instantaneous velocity  $v = \omega l = l (d\theta/dt)$ Hence,  $f_d = -kl (d\theta/dt)$ .

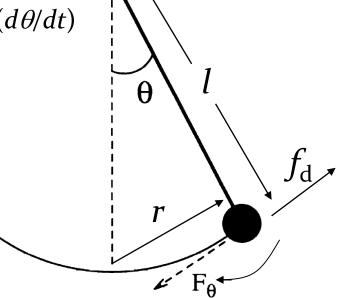
The net force on the forced pendulum along the tangential direction

$$F_{\theta} = -m g \sin \theta - kl (d\theta/dt).$$

$$F_{\theta} = -mg\sin\theta - kl\frac{d\theta}{dt} \approx -mg\theta - kl\frac{d\theta}{dt};$$

$$m \frac{d^{2}r}{d^{2}t} \approx m \frac{d^{2}}{dt^{2}} (l\theta) = m l \frac{d^{2}\theta}{dt^{2}};$$

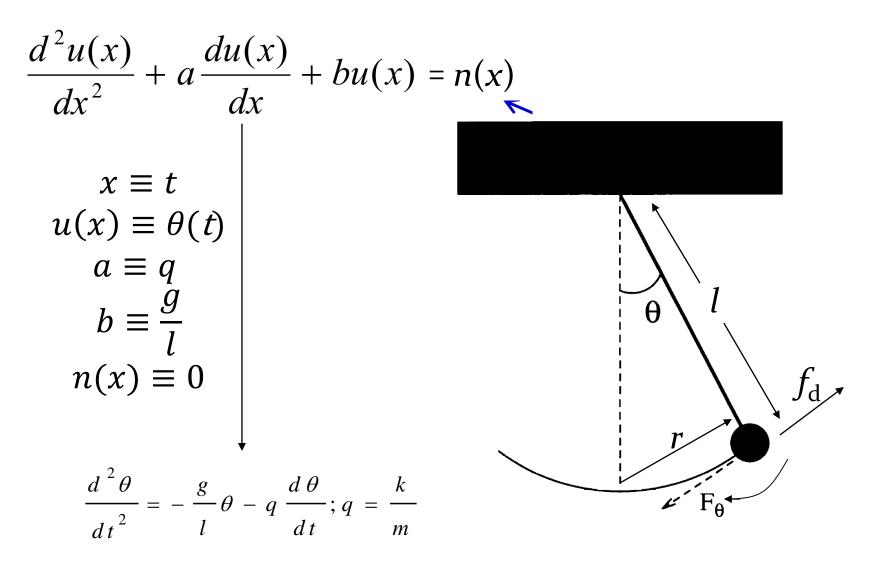
$$F_{\theta} = m \frac{d^{2}r}{d^{2}t} \rightarrow \frac{d^{2}\theta}{dt^{2}} = -\frac{g}{l}\theta - \frac{k}{m}\frac{d\theta}{dt} = -\frac{g}{l}\theta - q\frac{d\theta}{dt}; q =$$



k

m

### Simple Harmonic pendulum with drag force as a special case of second order DE (cont.)



#### Analytical solution

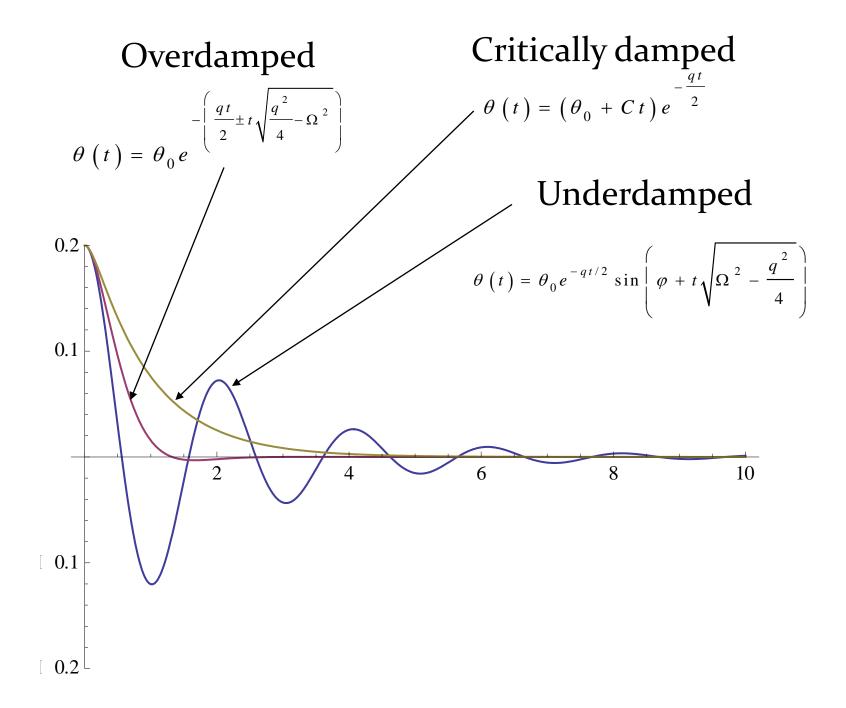
Underdamped regime (small damping). Still oscillate, but amplitude decay slowly over many period before dying totally.  $\theta(t) = \theta_0 e^{-qt/2} \sin\left(\varphi + t \sqrt{\Omega^2 - \frac{q^2}{4}}\right)$  $\Omega = \sqrt{\frac{g}{t}} \text{ the natural frequency of the system}$ 

Overdamped regime (very large damping), decay slowly over several period before dying totally.  $\theta$  is dominated by exponential term.  $-\left(\frac{qt}{2} \pm t\sqrt{\frac{q^2}{4} - \Omega^2}\right)$ 

$$\theta\left(t\right) = \theta_0 e$$

Critically damped regime, intermediate between under- and overdamping case.

$$\theta(t) = (\theta_0 + Ct)e^{-\frac{qt}{2}}$$



See <u>20DE</u> Pendulum.nb where **DSolve** solves the three cases of a damped pendulum analytically.

## Adding driving force to the damped oscillator: forced oscillator

 $F_{\theta} = -mg\sin\theta - kl(d\theta/dt) + F_D\sin(\Omega_D t) \qquad \begin{array}{l} \Omega_D \text{ frequency of} \\ \text{the applied force} \end{array}$ 

 $F_{\theta} = -mg\sin\theta - kl\frac{d\theta}{dt} + F_{D}\sin\left(\Omega_{D}t\right) \approx -mg\theta - kl\frac{d\theta}{dt} + F_{D}\sin\left(\Omega_{D}t\right);$ 

$$F_{\theta} = m \frac{d^2 r}{d^2 t} \approx m \frac{d^2}{dt^2} (l\theta) = m l \frac{d^2 \theta}{dt^2};$$

$$F_{\theta} = m \frac{d^{2}r}{d^{2}t} = m l \frac{d^{2}\theta}{dt^{2}} \approx -m g \theta - k l \frac{d\theta}{dt} + F_{D} \sin\left(\Omega_{D}t\right)$$

$$\frac{d^{2}\theta}{dt^{2}} \approx -\frac{g}{l}\theta - q\frac{d\theta}{dt} + \frac{F_{D}\sin\left(\Omega_{D}t\right)}{ml}; q = \frac{k}{m}$$

#### Analytical solution

$$\theta(t) = \theta_0 \sin(\Omega_D t + \phi)$$
$$\theta_0 = \frac{F_D / (ml)}{\sqrt{\left(\Omega^2 - \Omega_D^2\right)^2 + \left(q\Omega_D\right)^2}}$$

Resonance happens when  $\Omega_D = \Omega = \sqrt{g/l}$ 

# Forced oscillator: An example of non homogeneous 2<sup>nd</sup> order DE

$$\frac{d^{2}u(x)}{dx^{2}} + a\frac{du(x)}{dx} + bu(x) = n(x)$$

$$x \equiv t$$

$$u(x) \equiv \theta(t)$$

$$a \equiv q$$

$$b \equiv \frac{g}{l}$$

$$n(x) \equiv \frac{F_{D}\sin(\Omega_{D}t)}{ml}$$

$$\frac{d^{2}\theta}{dt^{2}} = -\frac{g}{l}\theta - q\frac{d\theta}{dt} + \frac{F_{D}\sin(\Omega_{D}t)}{ml}$$

### **Exercise: Forced oscillator**

$$\frac{d^{2}\theta}{dt^{2}} = -\frac{g}{l}\theta - q\frac{d\theta}{dt} + \frac{F_{D}\sin\left(\Omega_{D}t\right)}{ml}$$

Use DSolve to solve the forced oscillator. Plot on the same graph the analytical solutions of  $\theta(t)$  for t from 0 to 10 T, where  $T = 2\pi/\Omega$ ,  $\Omega = \sqrt{g/l}$ , for  $\Omega_D = 0.01\Omega$ ,  $0.5\Omega$ ,  $0.99\Omega$ ,  $1.5\Omega$ ,  $4\Omega$ . Assume the boundary conditions  $\theta(t=0)=0$ ;  $d\theta/dt(t=0)=0$ ;  $m=l=F_D=1$ ; q=0.

See forced\_Pendulum.nb.

Second order Runge-Kutta (RK2) method

Consider a generic second order differential equation.

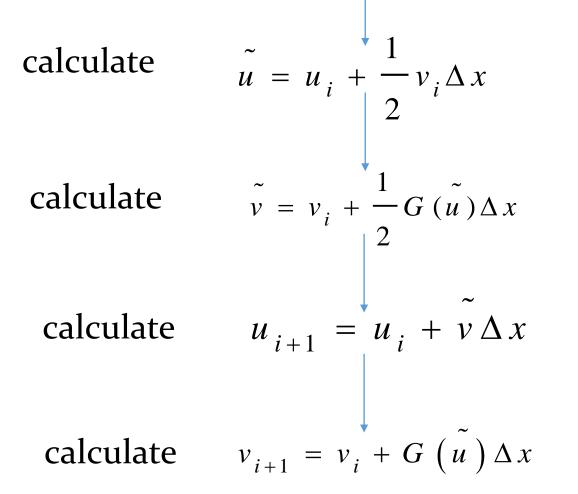
$$\frac{d^{2}u(x)}{dx^{2}} = G(u)$$

It can be numerically solved using second order Runge-Kutta method. First, split the second order DE into two first order parts:

$$v(x) = \frac{du(x)}{dx}$$
  $\frac{dv(x)}{dx} = G(u)$ 

### Algorithm

Set boundary conditions:  $u(x=x_o)=u_o$ ,  $u'(x=x_o)=v(x=x_o)=v_o$ .



#### Translating the SK2 algorithm into the case of simple pendulum $d^{2}u(x) = -\frac{g}{\theta}\theta(t)$ $\frac{d^{2}\theta(t)}{d^{2}\theta(t)} = -\frac{g\theta}{d^{2}\theta(t)}$

$$\frac{d^{2}u(x)}{dx^{2}} = G(u) \qquad G(u) =$$

$$v(x) = \frac{du(x)}{dx}$$

$$\frac{dv(x)}{dx} = G(u)$$

Set boundary conditions:  $u(x=x_o)=u_o, u'(x=x_o)=v(x=x_o)=v_o$ 

$$\tilde{u} = u_i + \frac{1}{2} v_i \Delta x$$

$$\tilde{v} = v_i + \frac{1}{2} G(\tilde{u}) \Delta x$$

$$u_{i+1} = u_i + \tilde{v} \Delta x$$

$$v_{i+1} = v_i + G(\tilde{u}) \Delta x$$

m into the case of  

$$\frac{d^{2}\theta(t)}{dt^{2}} = -\frac{g\theta}{l}$$

$$\omega(t) = \frac{d\theta(t)}{dt}$$

$$\frac{d\omega(t)}{dt} = -\frac{g\theta(t)}{l}$$
Set boundary conditions:  

$$\theta(t=t_{0}) = \theta_{0}, \theta'(t=t_{0}) = \omega(t=t_{0}) = \omega_{0}$$

$$\tilde{\theta} = \theta_{i} + \frac{1}{2}\omega_{i}\Delta t$$

$$\tilde{\omega} = \omega_{i} + \frac{1}{2}\left(-\frac{g\tilde{\theta}}{l}\right)\Delta t$$

$$\theta_{i+1} = \theta_{i} + \tilde{\omega}\Delta t$$

$$\omega_{i+1} = \omega_{i} + \left(-\frac{g\tilde{\theta}}{l}\right)\Delta t$$

Exercise: Develop a code to implement SK2 for the case of the simple pendulum. Boundary conditions:  $\omega(0) = \sqrt{\frac{g}{l}}; \theta(0) = 0$ 

See pendulum RK2.nb

## Translating the SK2 algorithm into the case of damped pendulum $d^2\theta(t) = g\theta$

$$\frac{du(x)}{dx^{2}} = G(u)$$

$$v(x) = \frac{du(x)}{dx}$$

$$\frac{dv(x)}{dx} = G(u)$$

$$G(u) = -\frac{g}{l}\theta(t) - q\omega(t)$$

Set boundary conditions:  
$$u(x=x_o)=u_o, u'(x=x_o)=v(x=x_o)=v_o$$
  
 $\sim 1$ 

$$u = u_{i} + \frac{1}{2} v_{i} \Delta x$$

$$\tilde{v} = v_{i} + \frac{1}{2} G(\tilde{u}) \Delta x$$

$$u_{i+1} = u_{i} + \tilde{v} \Delta x$$

$$v_{i+1} = v_{i} + G(\tilde{u}) \Delta x$$

$$\frac{l^2\theta(t)}{dt^2} = -\frac{g\theta}{l} - q\frac{d\theta}{dt}$$

$$\omega(t) = \frac{d\theta(t)}{dt}$$
$$\frac{d\omega(t)}{dt} = -\frac{g\theta}{l} - q\omega(t)$$

Set boundary conditions:  $\theta(t=t_{o})=\theta_{o}, \ \theta'(t=t_{o})=\omega(t=t_{o})=\omega_{o}$  $\tilde{\theta} = \theta_i + \frac{1}{2}\omega_i \Delta t$  $\tilde{\omega} = \omega_{i} + \frac{1}{2} \left( -\frac{g}{l} \tilde{\theta}(t) - q \tilde{\omega} \right) \Delta t \Rightarrow \tilde{\omega} = \frac{\left( \omega_{i} - \frac{g}{2l} \tilde{\theta}(t) \Delta t \right)}{\left( 1 + \frac{1}{2} q \Delta t \right)}$  $\theta_{i+1} = \theta_{i} + \tilde{\omega} \Delta t$  $\omega_{i+1} = \omega_i + \left( -\frac{g\theta}{l} - q\tilde{\omega} \right) \Delta t$ 

#### Exercise:

Develop a code to implement SK2 for the case of a pendulum experiencing a drag force, with damping coefficient  $q=0.1^*$  (4 $\Omega$ ),  $\Omega=\sqrt{g/l}, l=1.0$  m. Boundary conditions:  $\theta(0) = 0.2$ ;  $\omega(t=0) = 0$ ;

$$\frac{d^{2}\theta}{dt^{2}} = -\frac{g}{l}\theta - q\frac{d\theta}{dt}$$

#### Exercise:

Develop a code to implement SK2 for the case of a forced pendulum experiencing no drag force but a driving force  $F_D \sin(\Omega_D t)$ ,  $\Omega = \sqrt{g/l}$ , l = 1.0 m, m=1kg;  $F_D=1$ N;  $\Omega_D=0.99 \Omega$ ; Boundary conditions:  $\theta(0) = 0.0$ ;  $\omega(t = 0) = 0$ ;

$$\frac{d^{2}\theta}{dt^{2}} = -\frac{g}{l}\theta - q\frac{d\theta}{dt} + \frac{F_{D}\sin\left(\Omega_{D}t\right)}{ml}$$

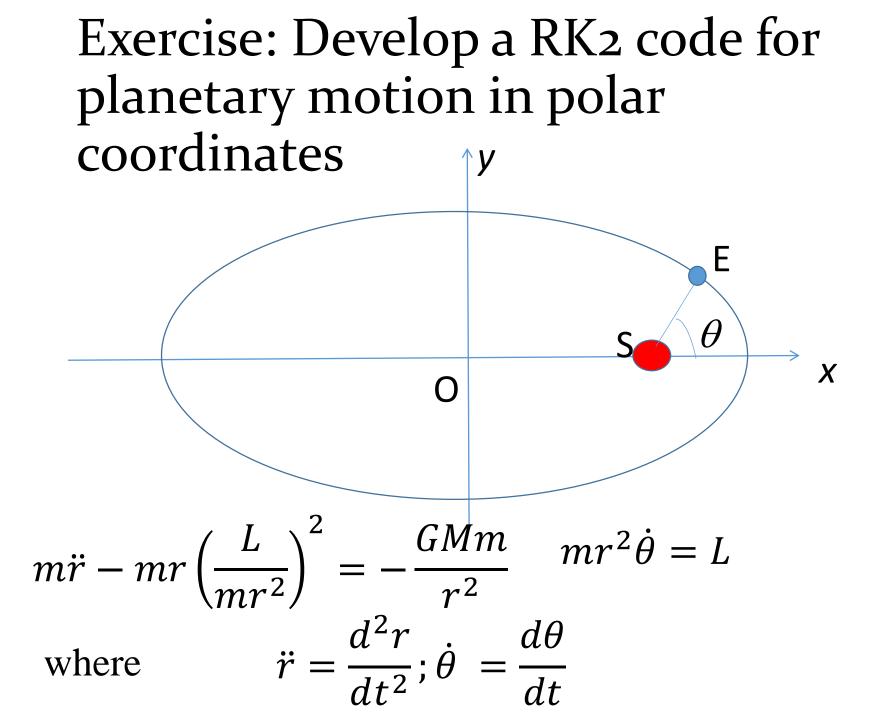
# Exercise: Stability of the total energy a SHO in RK2.

$$\omega = \frac{d\theta}{dt}$$
, angular velocity. *M*=1kg; *l*=1m.

The total energy of the SHO in can be calculated as

$$\begin{split} E_{i+1} &= K_{i+1} + U_{i+1} = \frac{1}{2}m\left(l\omega_{i+1}\right)^2 + mgl\left(1 - \cos\theta_{i+1}\right) \\ &\approx \frac{1}{2}ml^2\omega_{i+1}^2 + mgl\left[1 - \left(1 - \frac{\theta_{i+1}^2}{2}\right)\right] \\ &= \frac{1}{2}ml^2\omega_{i+1}^2 + \frac{1}{2}mgl\theta_{i+1}^2 \end{split}$$

User your RK2 code to track the total energy for *t* running from *t*=0 till t=25*T*;  $T=\sqrt{g/l}$ . Boundary conditions:  $\omega(0) = \sqrt{\frac{g}{l}}; \theta(0) = 0$  $E_i$  should remain constant throughout all  $t_i$ .



### Velocity verlet algorithm for solving the Newton second law

#### Newton's second law

•Given a position-dependent force acting on a particle, **F**(**r**), Newton second law determines the acceleration of a particle, **a**.

 $d^2r/dt^2 = F(r)/m$ 

- •This is a second order differential equation.
- •Given **F**(**r**), we wish to know what are the subsequent evolution of **r**(*t*), **v**(*t*) beginning from the boundary values of **r**(0), **v**(0).
- Previously we solve the second order DE using RK2 to obtain r(t), v(t).

#### Verlet algorithms

- The equation d<sup>2</sup>r/dt<sup>2</sup>=F(r)/m can be integrated to obtain r(t), v(t), via a numerical scheme: Verlet algoritm
- •Three types: ordinary Verlet, velocity Verlet, leap frog verlet.
- In the following, we shall denote the RHS as  $F(\mathbf{r})/m \rightarrow \mathbf{a}$ So that  $d^2\mathbf{r}/dt^2 = F(\mathbf{r})/m$   $\downarrow$  $d^2\mathbf{r}/dt^2 = \mathbf{a}$

See <u>http://en.wikipedia.org/wiki/Verlet\_integration</u>

#### Velocity Verlet algorithm

1. Calculate:

 $\vec{x}(t + \Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2$ 

- 2. Derive  $\vec{a}(t + \Delta t)$  from the interaction potential using  $\vec{x}(t + \Delta t)$
- 3. Calculate:

 $\vec{v}(t + \Delta t) = \vec{v}(t) + \frac{1}{2} \left( \vec{a}(t) + \vec{a}(t + \Delta t) \right) \Delta t$ 

Note, however, that this algorithm assumes that acceleration  $\vec{a}(t + \Delta t)$  only depends on position  $\vec{x}(t + \Delta t)$ , and does not depend on velocity  $\vec{v}(t + \Delta t)$ .

#### Global error in velocity Verlet algorithm

•The global (cumulative) error in x over a constant interval of time is given by

 $\Delta x \sim O(\Delta t^2)$ 

 Because the velocity is determined in a noncumulative way from the positions in the Verlet integrator, the global error in velocity is also

 $\Delta v \sim O(\Delta t^2)$ 

#### Exercise: SHO

- Solve for x(t), v(t), for a simple harmonic oscillator with constant k, mass m, initial displacement x<sub>0</sub>, and velocity v<sub>0</sub> =0, using velocity Verlet algorithm.
- For SHO,  $F = -kx \Rightarrow a = -(k/m)x$

$$d^2x/dt^2 = -(k/m)x$$

See <u>verlet\_algorithm\_samples.nb</u>

#### Exercise: 2D free-fall projectile

- •Solve for x(t), y(t), v(t) of a 2D free-fall projectile with initial speed  $v_0=0$  and launching angle  $\theta_0$ using velocity Verlet algorithm.
- •For 2D projectile motion,  $\mathbf{F} = -mg\hat{y} + 0\hat{x}$ .

$$\mathbf{a} = \mathbf{F}/m$$

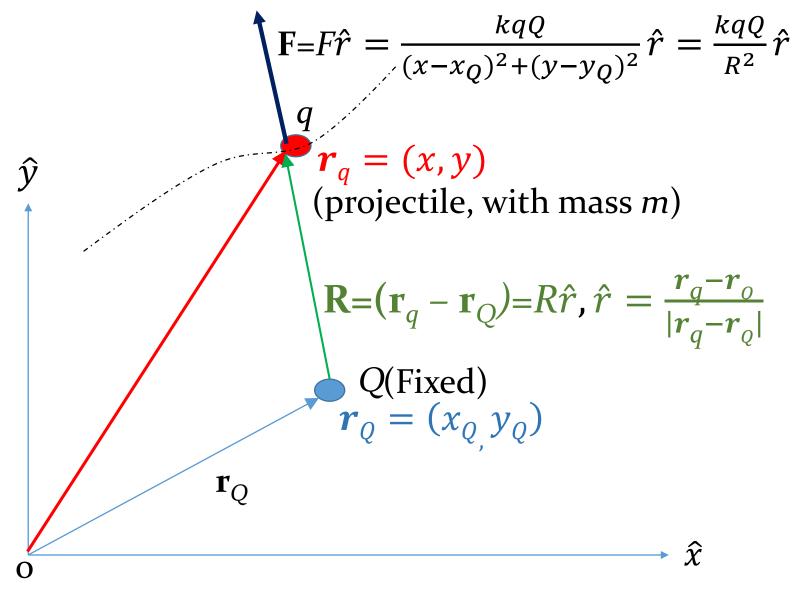
$$a_x \hat{x} + a_y \hat{y} = 0\hat{x} - g\hat{y}$$

$$d^2 x/dt^2 \hat{x} + d^2 y/dt^2 \hat{x} = -g\hat{y}$$

$$\Rightarrow d^2 x/dt^2 = 0, \quad d^2 y/dt^2 = -g$$

See <u>verlet\_algorithm\_samples.nb</u>

## Exercise: Scattering of a projectile charge via Coulomb force



Notation for scattering of a projectile charge via Coulomb force

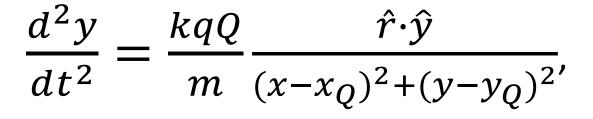
$$\mathbf{r}_{Q} = (x_{Q}, y_{Q}); \mathbf{r}_{q} = (x, y)$$

$$\mathbf{F} = k \frac{qQ}{(x - x_{Q})^{2} + (y - y_{Q})^{2}} \hat{r}; \quad \hat{r} = \frac{\mathbf{r}_{q} - \mathbf{r}_{Q}}{|\mathbf{r}_{q} - \mathbf{r}_{Q}|}$$

$$\mathbf{\bullet} \Rightarrow$$

# The equations required by Verlet algorithm

•
$$\boldsymbol{r}_{Q} = (\boldsymbol{x}_{Q}, \boldsymbol{y}_{Q}); \boldsymbol{r}_{q} = (\boldsymbol{x}, \boldsymbol{y}) \quad \hat{\boldsymbol{r}} = \frac{\boldsymbol{r}_{q} - \boldsymbol{r}_{Q}}{|\boldsymbol{r}_{q} - \boldsymbol{r}_{Q}|}$$



$$\frac{d^2x}{dt^2} = \frac{kqQ}{m} \frac{\hat{r} \cdot \hat{x}}{(x - x_Q)^2 + (y - y_Q)^2}$$

See verlet algorithm 2D coulomb scatterings.nb

# Störmer-Verlet integration algorithm

$$\vec{x}_{n+1} = 2\vec{x}_n - \vec{x}_{n-1} + \vec{a}_n(\Delta t)^2$$

$$\vec{v}_{n+1} = (\vec{x}_{n+1} - \vec{x}_n) / \Delta t$$

- Another variant of Verlet algoritm
- Use this for integrating dynamical system with a velocity-dependent acceleration, such as Lorentz force on a moving charge particle.
- The cumulative error in the velocity is larger than that in velocity Verlet algorithm

# Exercise: Charge moving in a magnetic field

- A charge (mass *m* and charge *q*) moving with velocity **v** = $(v_x, v_y, v_z)$  in a magnetic field **B**= $(B_x, B_y, B_z)$  experiences a velocity-dependent Lorentz force  $\mathbf{F} = (F_x, F_v, F_z) = q \mathbf{v} \times \mathbf{B}$ . Develop a code based on the Störmer-Verlet integration algorithm to simulate the dynamical path of the charge particle moving through the magnetic field. Assume: q=+1unit, mass m = 1 unit, initially located at (0,0,0), initial velocity ( $v_{0x}$ ,  $v_{0y}$ ,  $v_{0z}$ ),  $v_{0x}$ = $v_{0y}$ =0.1 unit,  $v_{0z}$ =0.05 unit,  $\mathbf{B}=(0, 0, B_{z}), B_{z}=0.1$  unit. You should see a helical trajectory circulating about the z-direction.
- verlet\_algorithm\_3D\_coulomb\_helix.nb