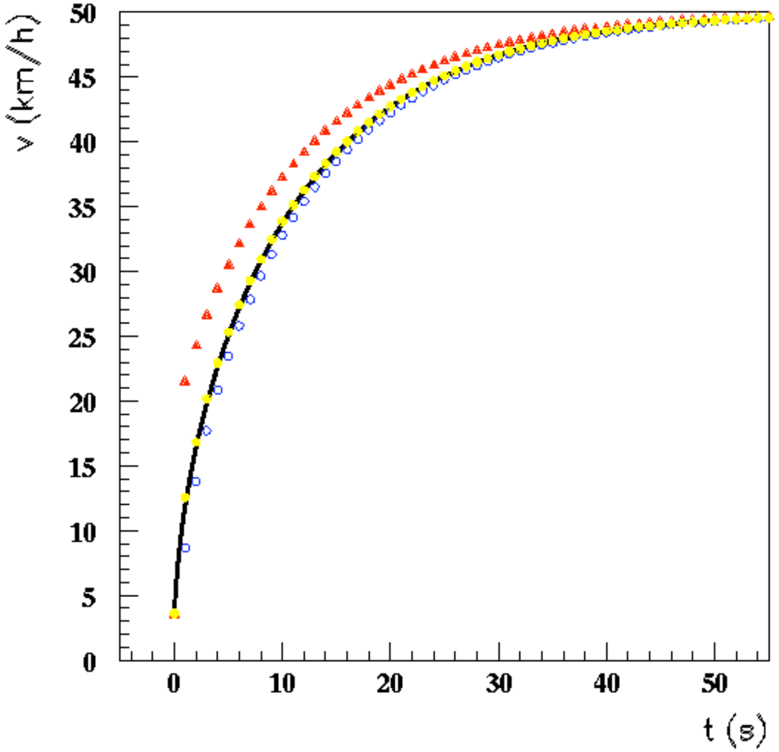
# *Numerical Algorithms for Differential Equations*

Topics: adaptive step size, higher derivatives, several dimensions




Last time, looked at bicycle rider example with different techniques. For this comparison, we took a fixed time step in all methods (1s). Can we do better with a variable step ?

- Exact
- Euler method
- 2nd order Runge-Kutta
- 4th order Runge-Kutta

## *Adaptive Step Size*

Let's try it out on the bike riding example and the 2nd order R-K method with a variable time step. Recall the 2nd order R-K technique:

$$x(t+\Delta t) = x(t) + f(x',t')\Delta t \quad \text{where} \quad \frac{dx}{dt} = f(x,t)$$

$$x' = x(t) + \frac{1}{2} f(x(t),t)\Delta t \qquad t' = t + \frac{1}{2}\Delta t$$

Substition showed: $$x(t+\Delta t) = x(t) + \frac{dx}{dt}\Delta t + \frac{1}{2}\frac{d^2 x}{dt^2}(\Delta t)^2$$

Comparison with Taylor series expansion shows that the error comes from missing terms with higher derivatives of *f* and higher powers of $\Delta$t. In adaptive step size methods, we take small $\Delta$t when derivatives are large, and vice-versa.

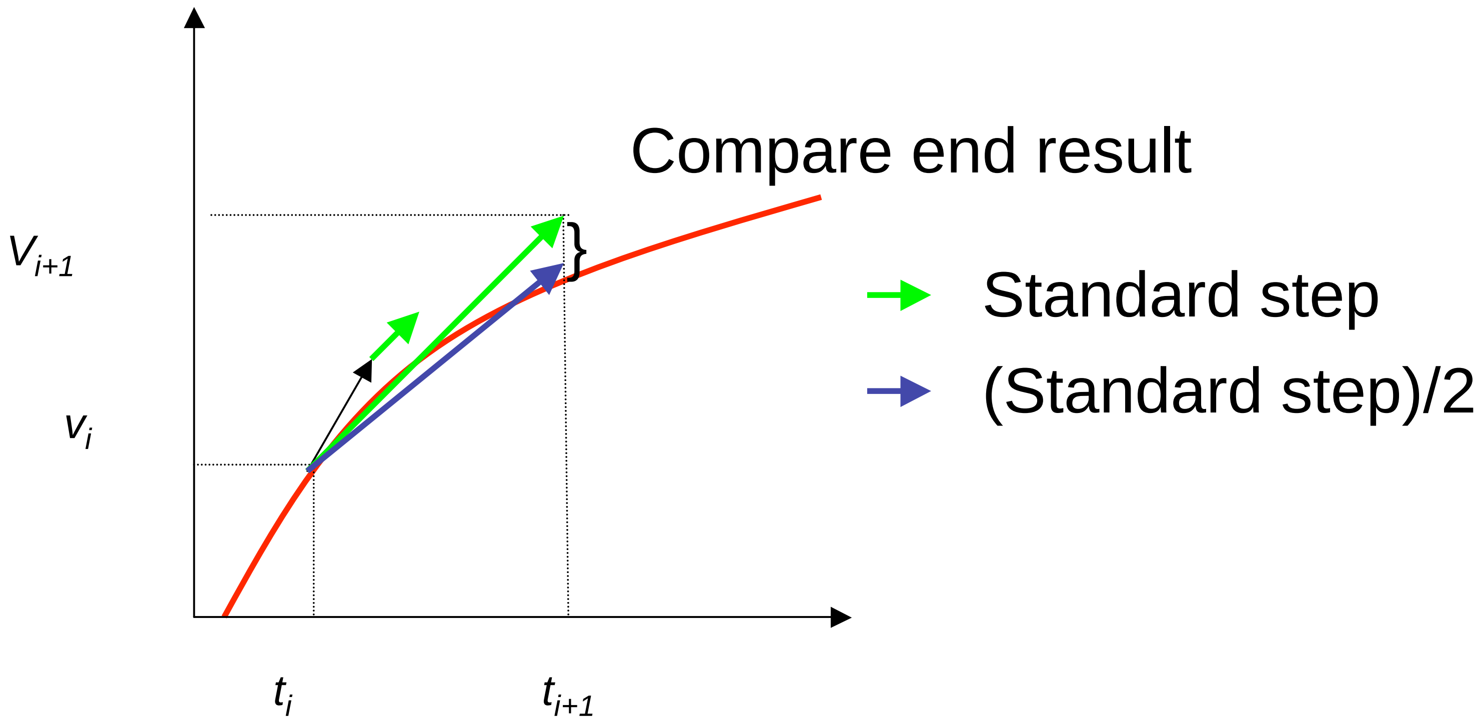
# *Adaptive Step Size*

Basic idea: take smaller steps when the function is changing rapidly. How do we know it is changing rapidly ? Evaluate with different $\Delta t$ and see what happens.

Typical Algorithm:

1. Update quantity of interest with current step size using your algorithm, call the result $y_1$
2. Take two steps each with 1/2 the current step size, call the result $y_2$
3. Compare $y_2, y_1$.
   - If the difference is greater than a maximum value, *eps,* then decrease the step, and go back to 1 (unless below minimum step size)
   - If the difference is within the requested resolution, accept the step and proceed to the next step but with a large step size.

# *Adaptive Step Size*

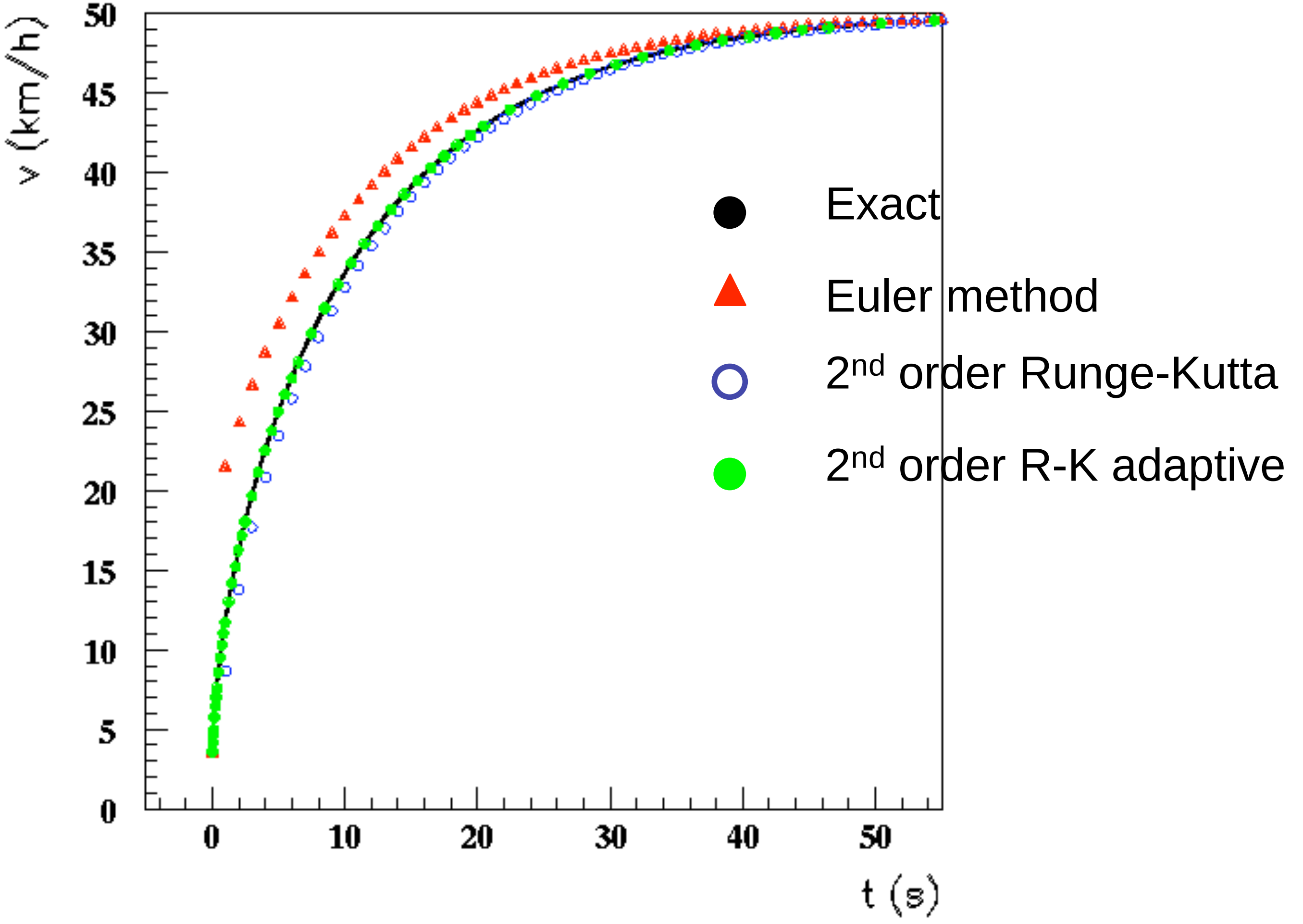


# *Adaptive Step Size*

```
      v=1.      ! Set the starting velocity
      t=0.      ! Set the starting time
      dt=1.     ! Set the starting step
 2    continue
* Calculate the intermediate velocity using the
* 2nd order R-K method
      vp=v+0.5*(P/(m*v)-(C*A*rho*v**2)/(2.*m))*dt
* Now the correction to the velocity
      dv1=(P/(m*vp)-(C*A*rho*vp**2)/(2.*m))*dt
* Now try with 1/2 the step size
 1    dt=dt/2.
      vp=v+0.5*(P/(m*v)-(C*A*rho*v**2)/(2.*m))*dt
      dv21=(P/(m*vp)-(C*A*rho*vp**2)/(2.*m))*dt
      v2=v+dv21
      vp=v2+0.5*(P/(m*v2)-(C*A*rho*v2**2)/(2.*m))*dt
      dv22=(P/(m*vp)-(C*A*rho*vp**2)/(2.*m))*dt
      dv2=dv21+dv22
* Get the velocity difference between the
* two estimates
       dv=abs(dv2-dv1)
      If (dv.gt.eps) then
* Check if at minimum step size
        If (dt.gt.2.*dtmin) then
* No, then take over 1/2 step result and
* Try again.
          dv1=dv21
          goto 1
        Else
* Yes, have to use this minimum step
* Use the finer step size for updating
          v=v+dv2
          t=t+2.*dt
* Reset the step size
          dt=2.*dt
        Endif
      Else
* Update
        v=v+dv2
        t=t+2.*dt
* Try larger step next time
        dt=4.*dt
      Endif
      If (t.le.total_t) goto 2
```

# *Adaptive Step Size*

Here we take *eps=0.001*, $\Delta t_{min}$*=0.001 s*



# *Adaptive Step Size*

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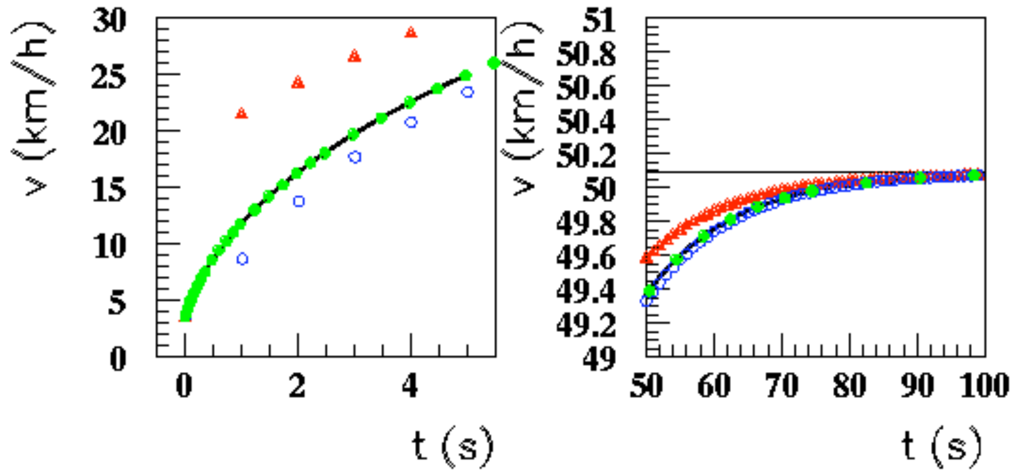
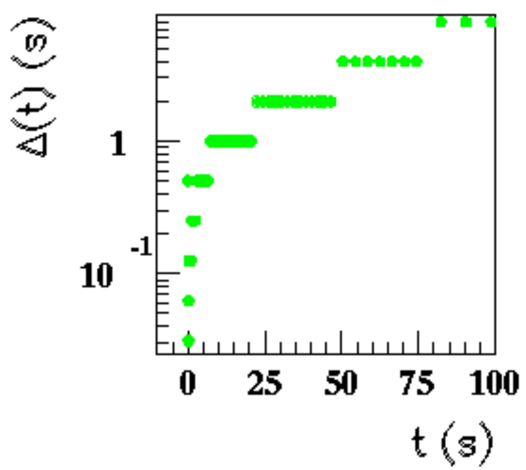



Many steps at small *t*, only a few at large *t*




Main advantages:

• desired accuracy can be chosen, rather than step

• can save considerable computer time since minimum step not used everywhere.

## *Higher Derivatives*

Method 1: Rewrite higher derivative as series of single derivatives:

$$\text{e.g.,}\quad \frac{d^2x}{dt^2} + q(t)\frac{dx}{dt} = r(t) \quad \text{can be rewritten as}$$

$$\frac{dx}{dt} = z(t) \qquad\qquad \frac{dz}{dt} = r(t) - q(t)z(t)$$

We then use our favorite method for the first-order equations twice. Take as an example the simple harmonic oscillator:

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x \qquad \frac{dv}{dt} = -\frac{k}{m}x \qquad \frac{dx}{dt} = v$$

Need to specify initial conditions:

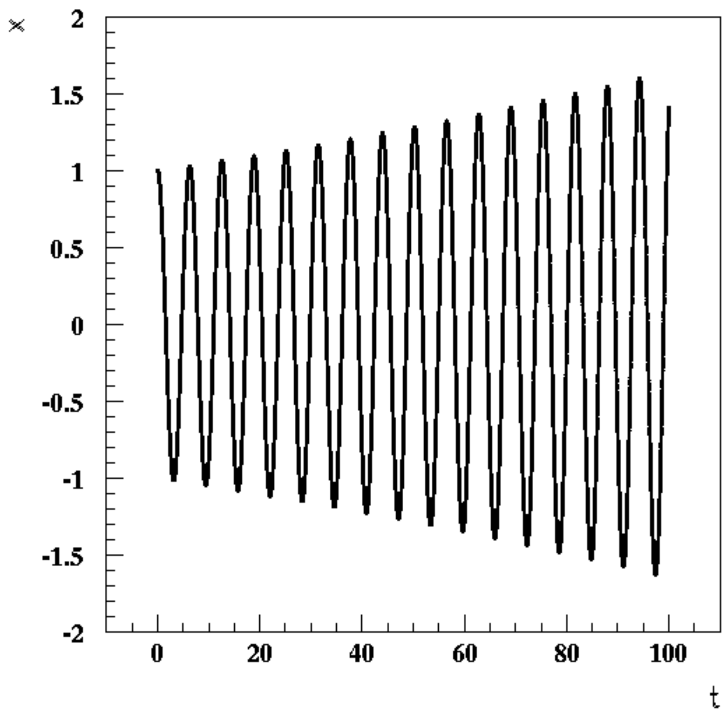
$$\text{e.g.,}\quad x_0 = 1 \quad v_0 = 0 \qquad \text{Let's also take} \quad \frac{k}{m} = 1$$

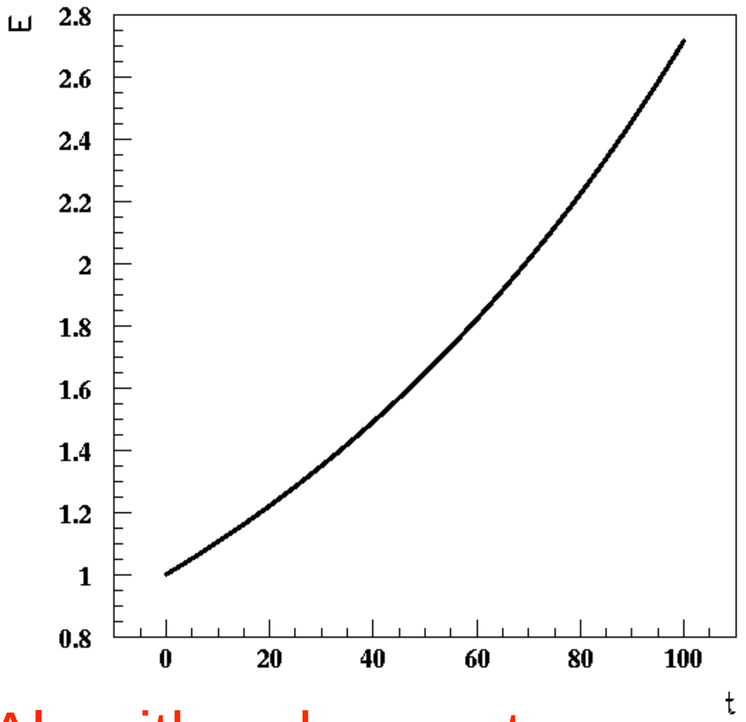
# *Higher Derivatives*

Start with the Euler Method:

$$v_{i+1} = v_i - \frac{k}{m} x_i \Delta t \qquad x_{i+1} = x_i + v_i \Delta t \qquad \text{Try } \Delta t = 0.01$$

What happened ?




Algorithm does not conserve energy !

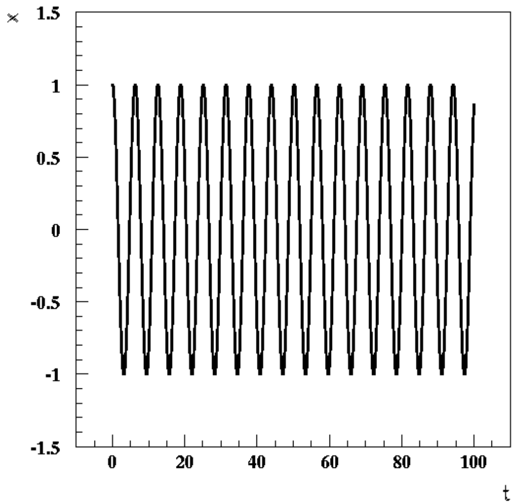
# *Harmonic Oscillator*

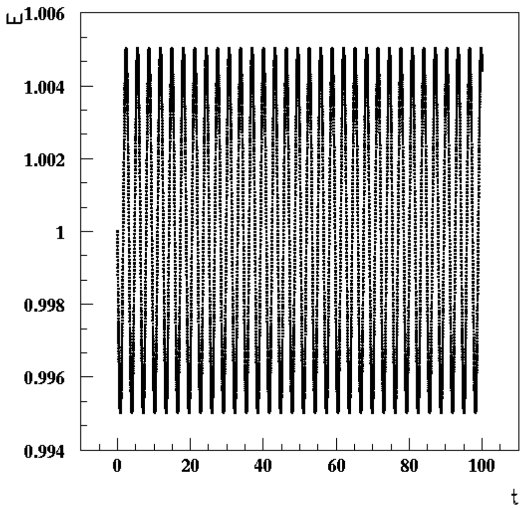
Now we make the simple change

$$\frac{dv}{dt} = -\frac{k}{m}x \qquad \frac{dx}{dt} = v$$

$$v_{i+1} = v_i - \frac{k}{m}x_i\Delta t \quad x_{i+1} = x_i + \boxed{v_{i+1}}\Delta t$$

Euler-Cromer




Discovered by accident !

This reminds us of the discussion from last lecture - different ways to estimate the average derivative in a step.

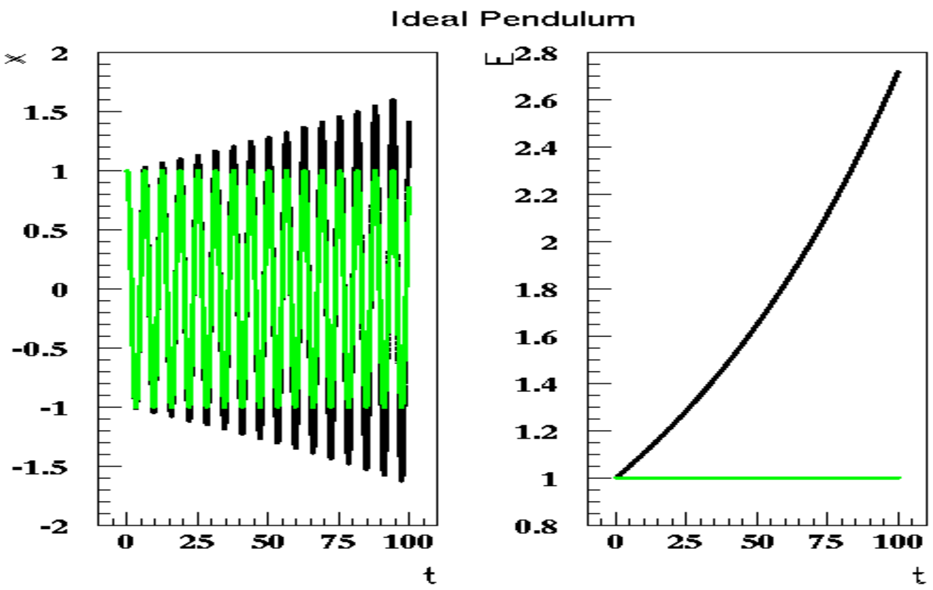
# *Harmonic Oscillator*

Let's try the 2nd order R-K method on the SHO:

$$x' = x(t) + \frac{1}{2} f_x(x,v,t)\Delta t \qquad v' = v(t) + \frac{1}{2} f_v(x,v,t)\Delta t \qquad t' = t + \frac{1}{2}\Delta t$$

$$v(t+\Delta t) = v(t) + f_v(x',v',t')\Delta t \qquad \text{where} \quad f_v(x,v,t) = -\frac{k}{m}x$$

$$x(t+\Delta t) = x(t) + f_x(x',v',t')\Delta t \qquad \text{where} \quad f_x(x,v,t) = v$$




—Euler Method

—2nd order R-K

## *Higher derivatives*

Let's us look at a different way to code higher derivatives:

$$\frac{d^2y}{dx^2}+q(x)\frac{dy}{dx}=r(x)$$

Method 2: try to evaluate second derivative directly - need at least three points to see the curvature.

Suppose have set of points $x_{-1},x_0,x_1$ and $y_{-1},y_0,y_1$

Lagrange polynomial interpolation:

$$p(x)=y_{-1}\frac{(x-x_0)(x-x_1)}{(x_{-1}-x_0)(x_{-1}-x_1)}+y_0\frac{(x-x_{-1})(x-x_1)}{(x_0-x_{-1})(x_0-x_1)}+y_1\frac{(x-x_{-1})(x-x_0)}{(x_1-x_{-1})(x_1-x_0)}$$

$$=y_{-1}\frac{(x-x_0)(x-x_1)}{2(\Delta t)^2}+y_0\frac{(x-x_{-1})(x-x_1)}{-(\Delta t)^2}+y_1\frac{(x-x_{-1})(x-x_0)}{2(\Delta t)^2}$$

# *Higher Derivatives*

Take derivatives of this polynomial:

$$p'(x) = y_{-1}\frac{2x - x_0 - x_1}{2(\Delta x)^2} + y_0\frac{2x - x_{-1} - x_1}{-(\Delta x)^2} + y_1\frac{2x - x_{-1} - x_0}{2(\Delta x)^2}$$

$$p''(x) = \frac{y_{-1} - 2y_0 + y_1}{(\Delta x)^2}$$

Now make the approximation: $y(x) \approx p(x)$

And

$$y'(x_0) \approx p'(x_0) = y_{-1}\frac{-\Delta x}{2(\Delta x)^2} + y_0\frac{0}{-(\Delta x)^2} + y_1\frac{\Delta x}{2(\Delta x)^2} = \frac{y(x_0 + \Delta x) - y(x_0 - \Delta x)}{2\Delta x}$$

$$y''(x_0) \approx p''(x_0) = \frac{y_{-1} - 2y_0 + y_1}{(\Delta x)^2} = \frac{y(x_0 - \Delta x) - 2y(x_0) + y(x_0 + \Delta x)}{(\Delta x)^2}$$

Similar construction for higher derivatives (need more points)

# *Harmonic Oscillator*

Let's try this construction on our harmonic oscillator example.

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x \quad \Rightarrow \quad x_{i+1} = 2x_i - x_{i-1} + \left(-\frac{k}{m}x_i\right)(\Delta t)^2$$

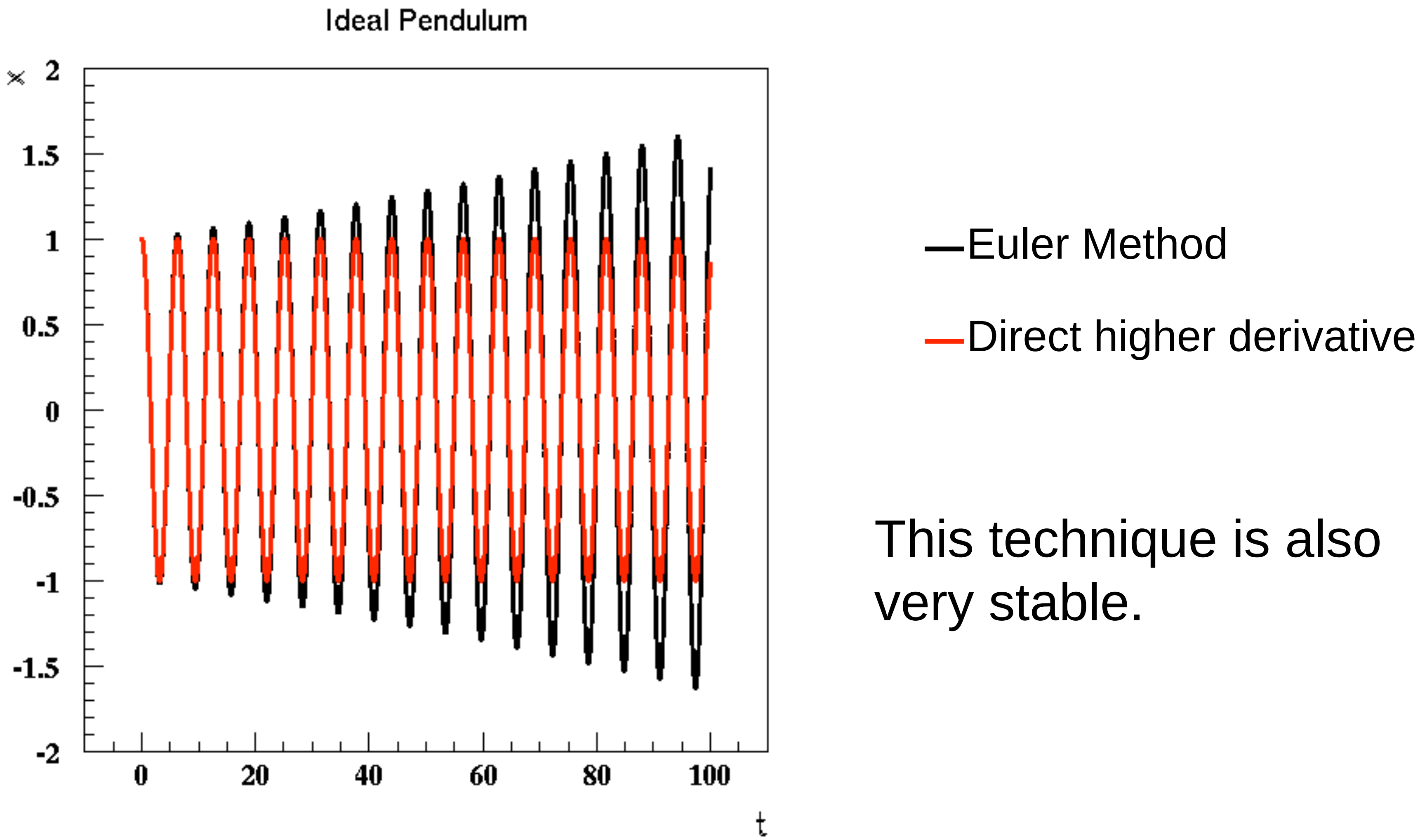
$$\text{Initial conditions: } x_0 = 1, \quad \left.\frac{dx}{dt}\right|_{t=0} = 0$$

Second condition gives

$$0 = x_1 - x_{-1}, \quad \text{so } 2x_{-1} = 2x_0 - \frac{k}{m}x_0(\Delta \mathrm{t})^2 \;,\; x_{-1} = 1 - \frac{(\Delta \mathrm{t})^2}{2}$$

With $x_0, x_{-1}$ defined, can start algorithm

# *Harmonic Oscillator*



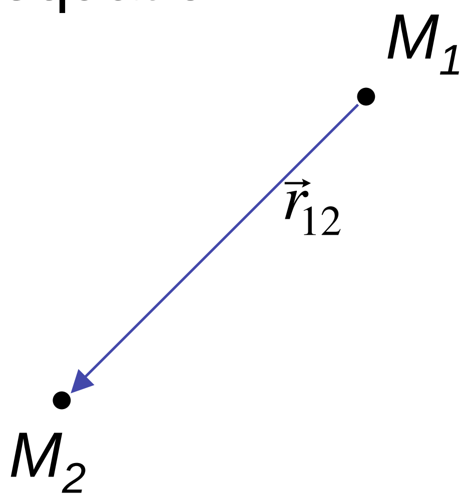

This technique is also very stable.

## *Several Dimensions*

So far, we have discussed first and higher order differential equations in a single variable. Let's look to see what happens when we have more than one variable. As an interesting example, we will look into planetary motion.

Of course, the basis of all this is Newton's equation:

$$\vec{F}_1 = \frac{GM_1M_2}{r^2}\hat{r}_{12}$$




The force along any direction is given by $\hat{e}\cdot\vec{F}$ where $\hat{e}$ is the unit vector in the direction of interest. E.g.,

$$F_x = \frac{GM_1M_2}{r^2}\hat{x}\cdot\hat{r} = \frac{GM_1M_2x}{r^3}$$ worry about sign later

# *Planetary Motion*

Start with two objects - the motion is in a plane. Also, assume for now that one object is much more massive than the other (e.g., Sun-Earth system). We put the massive object at the center of the coordinate system and look at the motion of the second object. Start with simple Euler approach.

$$\frac{dv_x}{dt} = -\frac{GMx}{r^3}$$

Here M is the mass of the Sun

$$\frac{dx}{dt} = v_x$$

$$\frac{dv_y}{dt} = -\frac{GMy}{r^3}$$

$$\frac{dy}{dt} = v_y$$

# Planetary Motion

Units: choice of units can make a problem easy or hard (don't want very small and very large numbers simultaneously because of rounding errors). From experience - be very careful with units !

$$\text{Circular motion}: \quad \frac{mv^2}{r} = \frac{GMm}{r^2}$$

$$\text{so } v^2 r = GM, \qquad v = \frac{2\pi r}{T} = 2\pi \quad \text{if T in years, r in A.U.}$$

$$\text{So we can write } GM = 4\pi^2$$

Write the differential equations as difference equations (Euler-Cromer algorithm)

$$v_{x,i+1} = v_{x,i} - \frac{4\pi^2 x_i}{r_i^3}\Delta t \qquad v_{y,i+1} = v_{y,i} - \frac{4\pi^2 y_i}{r_i^3}\Delta t$$

$$x_{i+1} = x_i + v_{x,i+1}\Delta t \qquad y_{i+1} = y_i + v_{y,i+1}\Delta t$$

# *Planetary Motion*

Here we treat the problem a little more carefully - go to polar coordinates. Note that for 2-body motion, motion has to be in a plane. For a force which depends only on the separation of the two objects, equivalent to one-body system, with position:

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\text{Reduced mass:} \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

Orbital trajectory for this object is given by:

$$\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right) + \frac{1}{r} = -\frac{\mu r^2}{L^2} F(r) \qquad L = \mu r^2 \dot{\theta} \ \text{(Angular Momentum)}$$

$F(r)$ is the force (keep general for now)

$L$ is conserved (no external torques)

# *Planetary Motion*

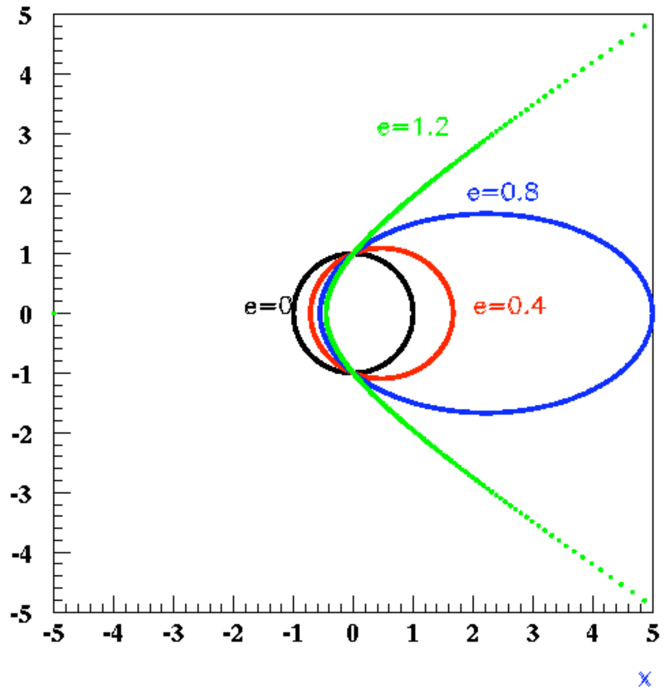
For $F(r) = \frac{GMm}{r^2}$ we get

$$\frac{1}{r} = \left(\frac{\mu GMm}{L^2}\right)[1 - e\cos(\theta + \theta_0)]$$

Taking $\theta_0 = 0$, we get

$$\boxed{r = \left(\frac{L^2}{\mu GMm}\right)\frac{1}{1 - e\cos\theta} \quad \text{conic section}}$$

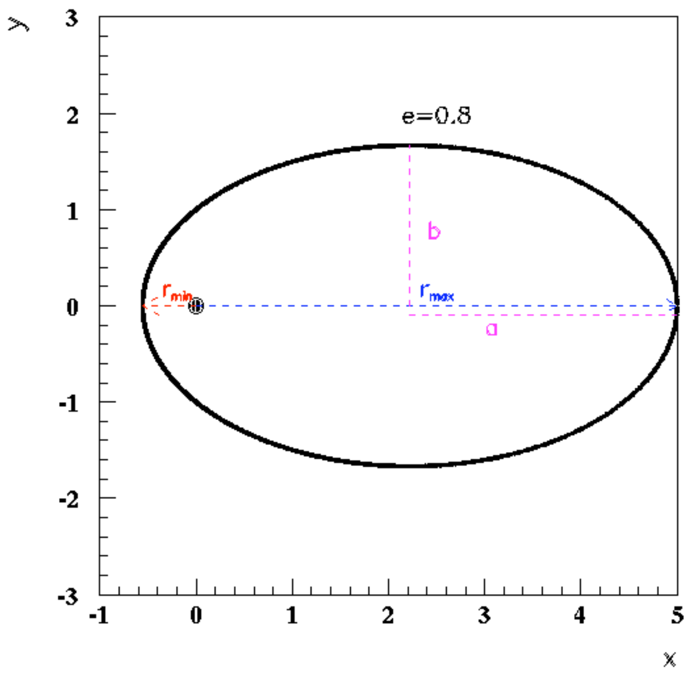
| | |
|---|---|
| *e=0* | circle |
| 0≤e<1 | ellipse |
| *e=1* | parabola |
| *e>1* | hyperbola |



# *Planetary Motion*

$$r = \left(\frac{L^2}{\mu GMm}\right)\frac{1}{1-e\cos\theta} \quad \text{for } \; e<1$$

$$r_{\max} = \left(\frac{L^2}{\mu GMm}\right)\frac{1}{1-e} = a(1+e) \quad r_{\min} = \left(\frac{L^2}{\mu GMm}\right)\frac{1}{1+e} = a(1-e)$$




$$a = \frac{r_{\min}+r_{\max}}{2} = \left(\frac{L^2}{\mu GMm}\right)\left(\frac{1}{1-e^2}\right)$$

$$b = \left(\frac{L^2}{\mu GMm}\right)\left(\frac{1}{\sqrt{1-e^2}}\right)$$

# *Planetary Motion*

$$a = \left(\frac{L^2}{\mu GMm}\right)\left(\frac{1}{1-e^2}\right) \quad \Rightarrow \quad L = \sqrt{\mu GMma(1-e^2)} \text{ conserved}$$

$$L = \mu r_{\min} v_{\max} = \mu r_{\max} v_{\min}, \text{ so}$$

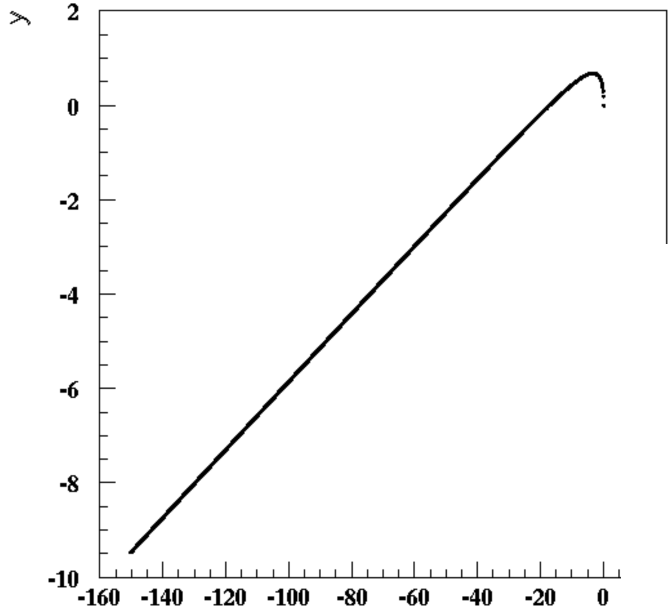
$$v_{\min} = \sqrt{GM}\sqrt{\frac{(1-e)}{a(1+e)}\left(1+\frac{m}{M}\right)}$$

$$v_{\max} = \sqrt{GM}\sqrt{\frac{(1+e)}{a(1-e)}\left(1+\frac{m}{M}\right)}$$

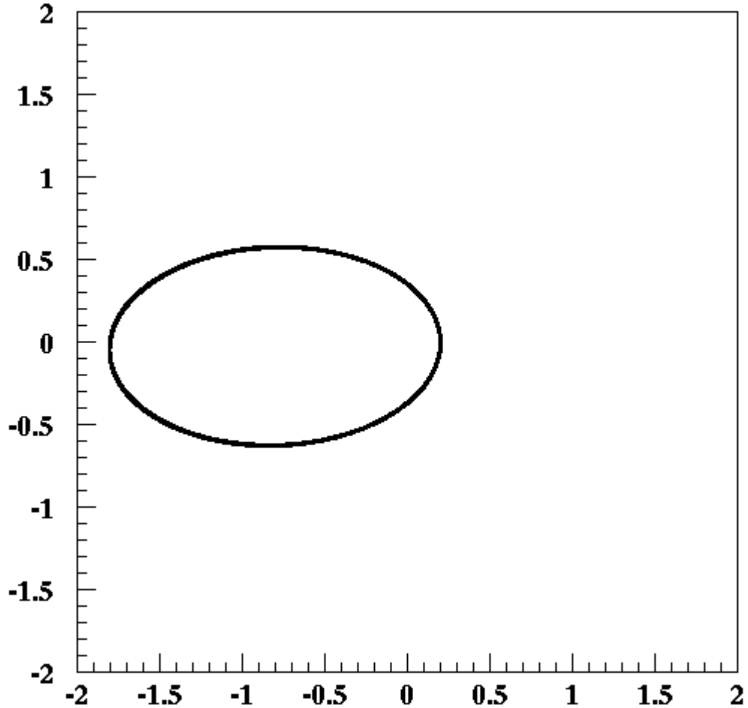
$$e.g., \; e = 0.8, \; GM = 4\pi^2 \text{ (AU)}, \; \frac{m}{M} = 1.\cdot 10^{-6}, \; a = 1$$

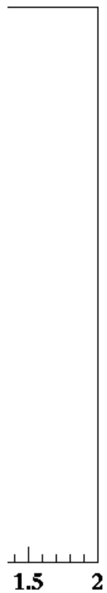
$$v_{\max} = 6\pi \quad v_{\min} = \frac{2\pi}{3} \quad b = a\sqrt{1-e^2} = 0.6$$

# *Planetary Motion*




With the Euler-Cromer method and step size 0.01




Runge-Kutta with ad
step size. Program
step about 0.0006 fc
eps=0.0001 . Try Eu
Cromer with this ste

# *Exercizes*

1. Write a program which takes an adaptive step size and try it out on the simple harmonic oscillator. Try different values of eps and see what happens.

2. Write a program for the simple harmonic oscillator using the $4^{th}$ order R-K algorithm. Compare the stability to the $2^{nd}$ order R-K method (look at long times, different step sizes).

3. For the planetary motion, take the force law to be $1/r^n$ with n=1.5,2.5,3 and plot some orbits. Next, try n=2.001 . Use an adaptive step size program with a small step.