Supporting textbook chapters for week 7: Chapters 8.4, 8.2, 8.5.5, 8.6

Lecture 7, topics:

- Adaptive step size for RK schemes,
- Bulirsch-Stoer method,
- Boundary value problems,
- Stability issues.

Last week: ODE(s) with some initial condition(s):

- 1D: $\dfrac{\mathrm{d}x}{\mathrm{d}t} = f(x, t) \quad \text{with} \quad x(t=0) = x_0.$
- nD: $\dfrac{\mathrm{d}x_i}{\mathrm{d}t} = f_i(x_1, \dots, x_n, t) \quad \text{with} \quad x_i(t=0) = x_{i0}.$
- higher order, e.g.:
$$\frac{\mathrm{d}^3 x}{\mathrm{d}t^3} = f(x, t) \quad \Leftrightarrow \quad \frac{\mathrm{d}x}{\mathrm{d}t} = v,\ \frac{\mathrm{d}v}{\mathrm{d}t} = a,\ \frac{\mathrm{d}a}{\mathrm{d}t} = f.$$

RK2:

- ⊕ Easily(sh) extended to RK4
- ⊕ Possible to use adaptive time step (this week)
- ⊖ time-reversible
- ⊖ accuracy

RK4:

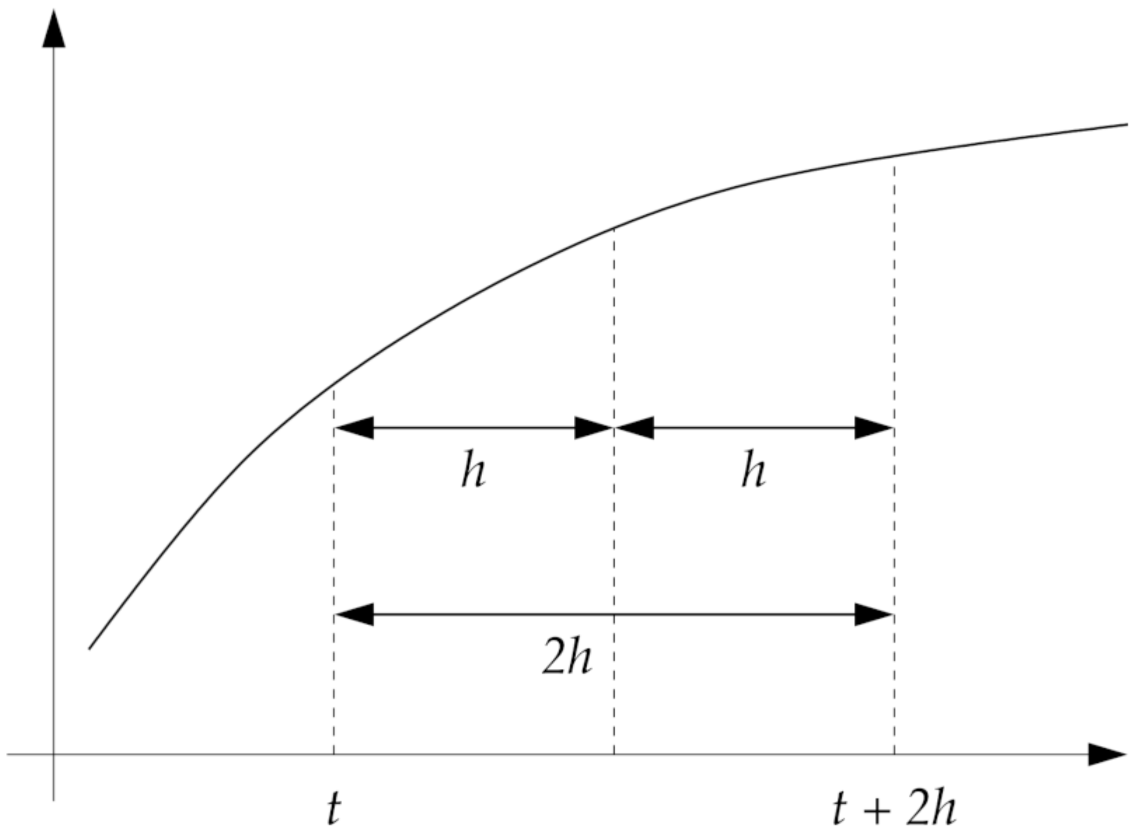
- ⊕ accuracy
- ⊕ Possible to use adaptive time step (this week)
- ⊖ time-reversible

Leapfrog:

- ⊕ time-reversible
- ⊕ basis for higher-order methods (Bulirsch-Stoer, this week)
- ⊖ accuracy
- ⊖ time step has to be constant (not exactly true, as we will see).

Error of RK4

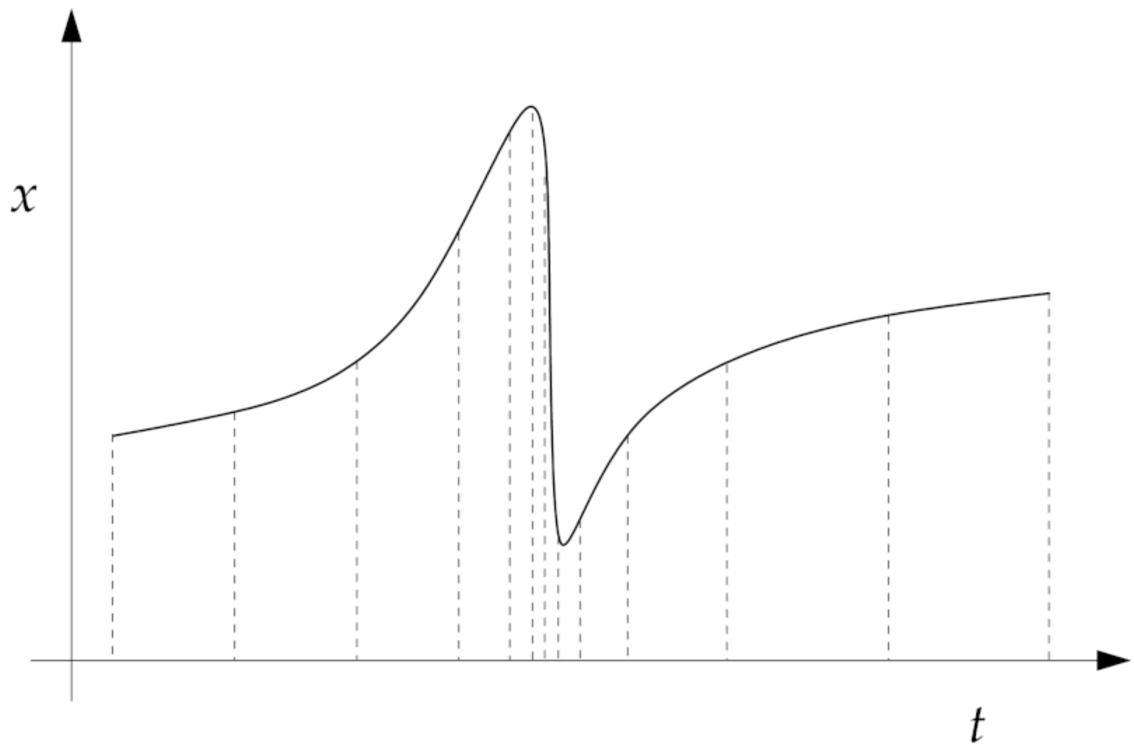
- Very accurate method: error is $\epsilon = ch^5$ at each time step h, c constant (order h^4 globally).
- Error after 2 time steps: $\approx 2ch^5$.
- Error after 1 time step of $2h$: $\approx c(2h)^5 = 32ch^5 \gg 2ch^5$
- The difference is $(32-2)ch^5 = 30ch^5 = 30\epsilon$.
- To estimate error: run ODE solver twice with h (to get x_1), once with $2h$ (to get x_2), divide difference by 30.
$$\epsilon = ch^5 = \frac{1}{30}(x_1 - x_2).$$



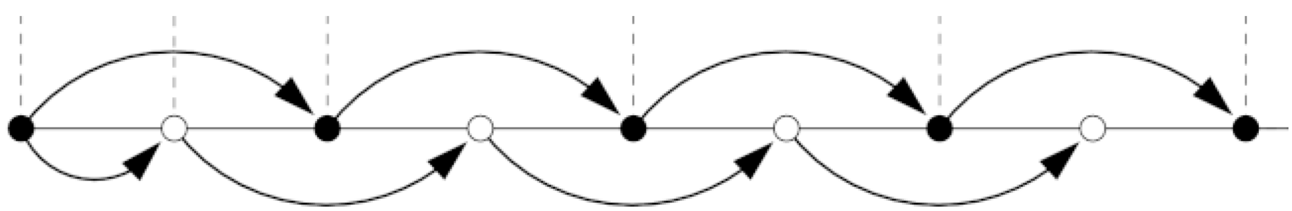
Adaptive time stepping

- Suppose target error is δ *per unit time* (physical time, not step).
- If
$$\rho = \frac{h\delta}{\epsilon} = \frac{30h\delta}{|x_1 - x_2|} = \frac{30\delta}{ch^4} > 1,$$
then h is too small (as in, could be bigger, saving computational resources while still reaching target accuracy) and can be adjusted to $h' = h\rho^{1/4}$ to get $\rho' = 1$.
    - Still achieves target error, which is $h'\delta$ for step of size h'.
    - Saves calculation time.

- If $\rho < 1$, the time step is too large and needs to be adjusted down by the same factor.
    - We also need to repeat our calculation to get the desired accuracy.
    - This will guarantee meeting error target.
- We test if we need to adjust by performing the calculation twice (we retrieve x_1 and x_2), testing if we met the target, and adjusting h.
- Overall, despite extra work (up to 3 RK4 steps per time step), program often faster because resolution focused where it's needed.



From Leapfrog to Bulirsch-Stoer



Leapfrog error

- Leapfrog is timestep-reversible.
- ⇒ error ϵ is an **odd** function of h:

$$\epsilon(-h) = -\epsilon(h)$$

  ⇒ Taylor expansion is made of **odd** powers of h,

$$\epsilon(h) = c_3 h^3 + c_5 h^5 + \ldots$$

- ⇒ cumulative error is **even** in h.
- Each improvement we apply ⇒ we can get two orders of accuracy, if we play it right.
- But first, we have to eliminate all even powers in ϵ due to first 1/2 step.

Modified mid-point (MMP) method

How to eliminate even powers of ϵ during the first 1/2 step?

- Integration from t to $t + H$, with $n + 1$ time steps:

$$\begin{aligned} x_0 &= x(t) \\ x_{1/2} &= x_0 + hf(x_0, t)/2 \quad \text{(Initial Euler 1/2-step} \Rightarrow \text{lots of even powers in } \epsilon!) \\ x_1 &= x_0 + hf(x_{1/2}, t + h/2) \\ x_{3/2} &= x_{1/2} + hf(x_1, t + h) \\ &\vdots \end{aligned}$$

- ... and keep going until you reach the end.
- So far, this is identical to Leapfrog.

- Then, do **both** the whole integer **and** the forward Euler 1/2-step.

$$x_{n-1/2} = x_{n-3/2} + hf(x_{n-1}, t + H - h),$$
$$x_n = x_{n-1} + hf(x_{n-1/2}, t + H - h/2) \approx x(t + H)$$
$$x_n' = x_{n-1/2} + hf(x_n, t + H) \approx x(t + H)$$

- Now do the following adjustment:
$$x(t + H)_{final} = \frac{x_n + x_n'}{2}$$
... and you have canceled the even powers (MMP method).

This is not a trivial result (cf. Gragg 1965 for proof; https://doi.org/10.1137/0702030 (https://doi.org/10.1137/0702030) PDF posted on Quercus if you're curious).

Bulirsch-Stoer method

MMP method rarely used by itself, but is the basis for the powerful Bulirsch-Stoer method:

- Take 1 single MMP step of size $h_1 = H$ to get estimate of
$$x(t + H) = R_{1,1}.$$
(R stands for "Richardson extrapolation")
- Now take 2 MMP steps of size $h_2 = H/2$ to get second estimate of
$$x(t + H) = R_{2,1}.$$

- Since we know the MMP has 2nd order and even total error, we can write both of these estimates as
$$x(t + H) = R_{1,1} + c_1 h_1^2 + O(h_1^4) \quad \text{and}$$
$$x(t + H) = R_{2,1} + c_1 h_2^2 + O(h_2^4).$$
- Using the relationship between the step sizes: $h_1 = 2h_2$, we can equate these expressions to get
$$R_{1,1} + 4c_1 h_2^2 + O(h_2^4) = R_{2,1} + c_1 h_2^2 + O(h_2^4)$$
$$\Rightarrow \; c_1 h_2^2 = \frac{1}{3}(R_{2,1} - R_{1,1}) + O(h_2^4).$$
- If we plug this back in to the expression for $x(t + H)$ above we get a new estimate called $R_{2,2}$:
$$x(t + H) \approx R_{2,2} + \boxed{O(h_2^4)}$$

$$x(t+H) = \underbrace{R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1})}_{R_{2,2}} + \boxed{O(h_2^4)}.$$

- 2 different grid spacings (H and $H/2$) → expression for the leading error term → replace it with our estimates for these grid spacings, i.e., $R_{1,1}$ and $R_{2,1}$.
- We have reduced the error in our estimate by 2 orders! *(which was possible because the errors were even)*

Why stop there?

- Take another grid spacing, to estimate the **new** leading order error term and then replace by that.
- E.g., with $h_3 = H/3$, MMP method yields
$$x(t + H) = R_{3,1} + c_1 h_3^2 + O(h_3^4).$$

- E.g., with $h_3 = H/3$, compare with estimate with $h_2 = H/2 = 3h_3/2$:
$$x(t + H) = R_{3,1} + c_1 h_3^2 + O(h_3^4),$$
$$= R_{2,1} + c_1 \left(\frac{3}{2}h_3\right)^2 + O(h_3^4),$$
$$\Rightarrow \; R_{3,1} + c_1 h_3^2 + O(h_3^4) = R_{2,1} + c_1 \frac{9}{4} h_3^2 + O(h_3^4)$$
$$\Rightarrow \; c_1 h_3^2 = \frac{4}{5}(R_{3,1} - R_{2,1}) + O(h_3^4)$$
- Now plugging this into our expression for $x(t + H)$ and calling it $R_{3,2}$,
$$x(t + H) \approx R_{3,2} + c_2 h_3^4 + \boxed{O(h_3^6)},$$
$$\text{where } R_{3,2} = R_{3,1} + \frac{4}{5}(R_{3,1} - R_{2,1}),$$

- Equating $R_{3,2}$ and $R_{2,2}$ allows to find c_2:

$$x(t+H) \approx R_{2,2} + c_2 h_2^4 + \boxed{O(h_2^6)}$$
$$\approx R_{3,2} + c_2 h_3^4 + \boxed{O(h_3^6)}$$
$$h_3 = 2h_2/3 \Rightarrow c_2 h_3^4 = \frac{16}{65}(R_{3,2} - R_{2,2})$$

- Plugging this back in and calling the new result $R_{3,3}$ yields

$$x(t+H) \approx R_{3,3} + O(h_3^6),$$
$$\text{where } R_{3,3} = R_{3,2} + \frac{16}{65}(R_{3,2} - R_{2,2}),$$

- and so on.

- The power in this method is that you keep cancelling 2 powers in the error for every new grid spacing you consider.
- Can continue the refinement until you reach the error tolerance you want.
- Summary of method:
  - Take $h = H$, set $n = 1$ and use MMP to find $x(t+H)$,
  - Continue to refine grid to find new estimates and error estimates.
  - When error is acceptable, stop.
- The iteration can be expressed:

$$x(t+H) = R_{n,m+1} + O(h_n^{2m+2}), \qquad \text{where}$$
$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1} \quad \text{and} \quad h_n = \left(\frac{n-1}{n}\right) h_{n-1}.$$

Look at `bulirsch.py` from textbook. for solving nonlinear pendulum,

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega, \qquad \frac{\mathrm{d}\omega}{\mathrm{d}t} = -\frac{g}{\ell}\sin\theta.$$

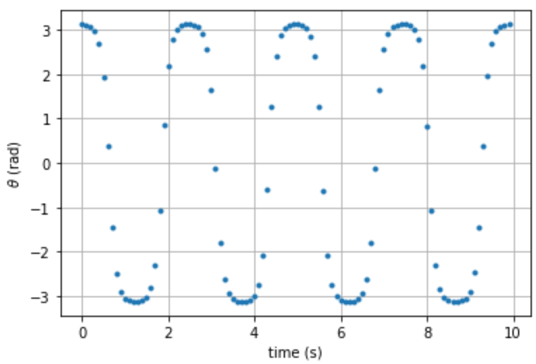
Extrapolation table:

$$\begin{array}{lccccccc}
n=1: & R_{1,1} & & & & & & \\
 & & \searrow & & & & & \\
n=2: & R_{2,1} & \rightarrow & R_{2,2} & & & & \\
 & & \searrow & & \searrow & & & \\
n=3: & R_{3,1} & \rightarrow & R_{3,2} & \rightarrow & R_{3,3} & & \\
 & & \searrow & & \searrow & & \searrow & \\
n=4: & \underbrace{R_{4,1}}_{MMP} & \rightarrow & R_{4,2} & \rightarrow & R_{4,3} & \rightarrow & R_{4,4}
\end{array}$$

In [8]:
```python
# adapted from bulirsch.py from Newman
from math import sin, pi
from numpy import empty, array, arange
from pylab import plot, show, xlabel, ylabel, figure, grid

g = 9.81
ell = 0.1
theta0 = 179*pi/180
a = 0.0
b = 10.0
N = 100  # Number of "big steps"
H = (b-a)/N  # Size of "big steps"
delta = 1e-8  # Required position accuracy per unit time

def f(r):
    theta = r[0]
    omega = r[1]
    ftheta = omega
    fomega = -(g/ell)*sin(theta)
    return array([ftheta, fomega], float)


tpoints = arange(a, b, H)
thetapoints = []
r = array([theta0, 0.0], float)
```

In [9]:
```
for t in tpoints: # Do the "big steps" of size H
    thetapoints.append(r[0])
    n = 1     # Do one modified midpoint step to get things started
    r1 = r + 0.5*H*f(r)
    r2 = r + H*f(r1)
    # array R1: row1 of extrapolation table, which contains the single MMP estimate for end of interval
    R1 = empty([1, 2], float)
    R1[0] = 0.5*(r1 + r2 + 0.5*H*f(r2))
    error = 2*H*delta # Now increase n until the required accuracy is reached
    while error > H*delta:
        n += 1
        h = H/n
        r1 = r + 0.5*h*f(r) # MMP
        r2 = r + h*f(r1)
        for i in range(n-1):
            r1 += h*f(r2)
            r2 += h*f(r1)
        R2 = R1*1 # Extrapolation estimates: Arrays R1, R2 hold the two most recent lines of the table
        R1 = empty([n, 2], float)
        R1[0] = 0.5*(r1 + r2 + 0.5*h*f(r2))
        for m in range(1, n):
            epsilon = (R1[m-1]-R2[m-1])/((n/(n-1))**(2*m)-1)
            R1[m] = R1[m-1] + epsilon
        error = abs(epsilon[0])  # epsilon[0] is theta error
    r = R1[n-1] # Set r to our most accurate estimate, before giong to next big step
```

In [12]:
```
# Plot the results
# plot(tpoints, thetapoints)
plot(tpoints, thetapoints, ".")
xlabel('time (s)')
ylabel(r'$\theta$ (rad)')
grid()
show()
```

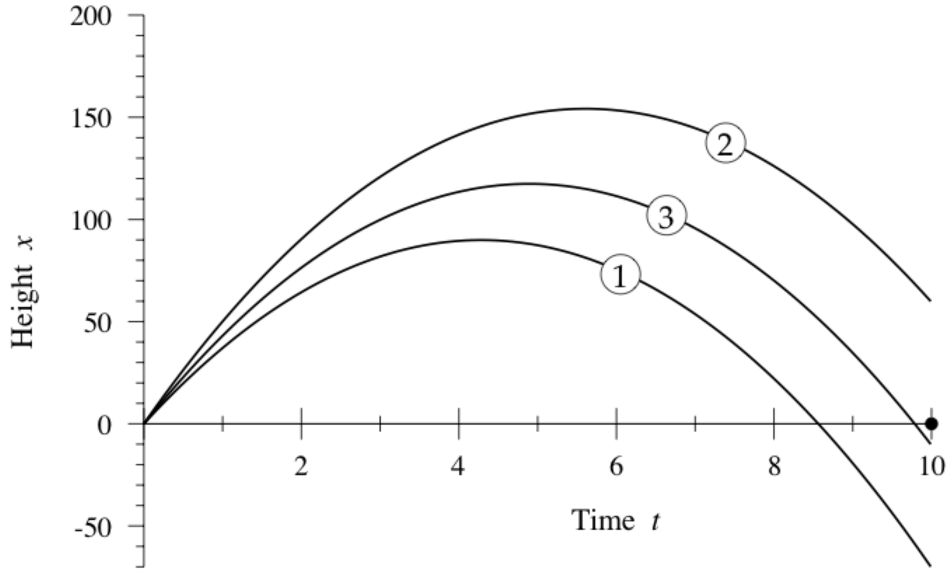


- Notes: This only calculates really accurate values for $x(t+H)$, not the region in between.
- Common practice (helps with efficiency/speed):
  - If your solution doesn't reach your tolerance level in some `nmax` steps (usually `nmax` $\sim 8-10$), half your interval and redo in smaller H regions.
  - Iterate until your regions are small enough that you reach the tolerance level in `nmax` steps: ``adaptive" method!

Boundary Value Problems

Shooting method

- Suppose we wanted to choose an initial velocity v_0 for a projectile to land after $t_L = 10$ s.
- $x(v_0, t)$ is a nonlinear function of v_0, and finding $x(v_0, t = t_L)$ can be done using root finding method (binary search, secant...)
- **Shooting method:** integrate the equations and adjust v_0 until you locate root.



In [15]:
```
# Based on Newman's throw.py
from numpy import array, arange

g = 9.81  # Acceleration due to gravity
a = 0.0  # Initial time
b = 10.0  # Final time
N = 1000  # Number of Runge-Kutta steps
h = (b-a)/N  # Size of Runge-Kutta steps
target = 1e-10  # Target accuracy for binary search

def f(r): # for Runge-Kutta calculation
    # [0] = v_x , [1] = a_x
    return array([r[1], -g], float)

def height(v): # to solve the equation and calculate final height
    # v = initial v_x, r[0] = x, r[1] = v_x
    r = array([0.0, v], float)
    for t in arange(a, b, h):
        k1 = h*f(r)
        k2 = h*f(r+0.5*k1)
        k3 = h*f(r+0.5*k2)
        k4 = h*f(r+k3)
        r += (k1+2*k2+2*k3+k4)/6
    return r[0]
```

In [16]:
```
# Main program performs a binary search
v1 = 0.01
v2 = 1000.0
h1 = height(v1)
h2 = height(v2)

while abs(h2-h1) > target:
    vp = (v1+v2)/2
    hp = height(vp)
    if h1*hp > 0:
        v1 = vp
        h1 = hp
    else:
        v2 = vp
        h2 = hp

v = (v1+v2)/2
print("The required initial velocity is", v, "m/s")
```

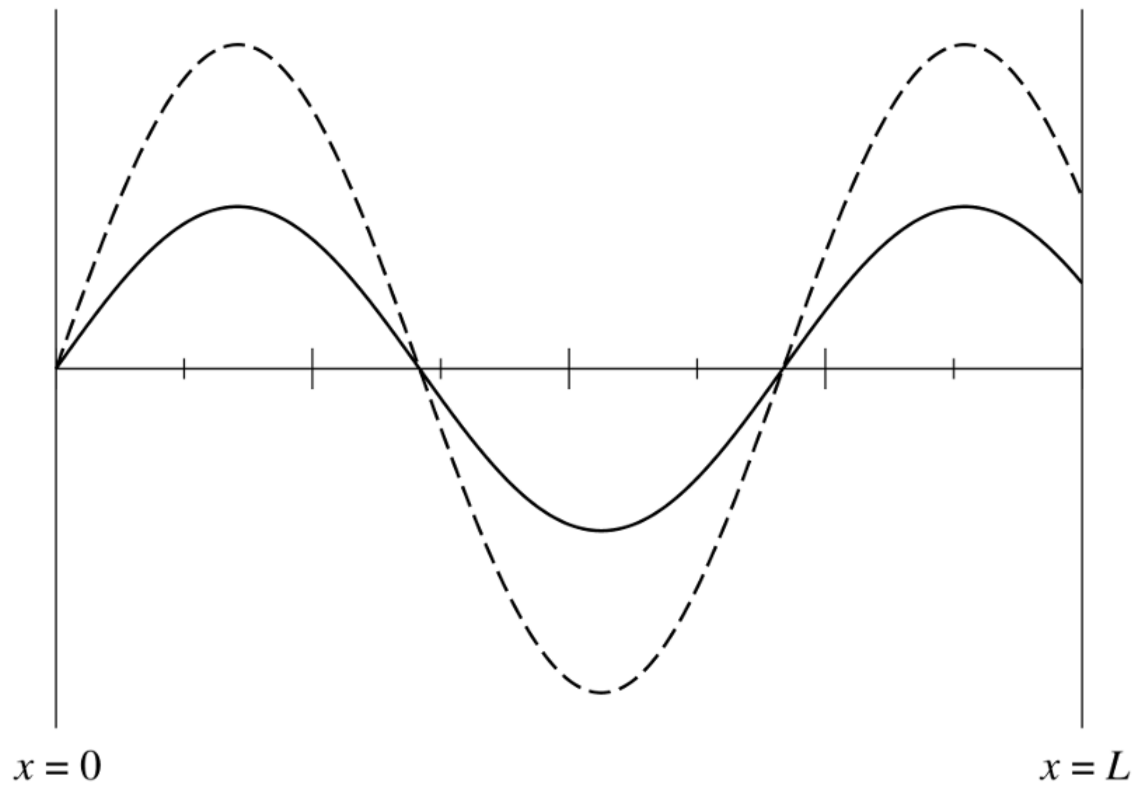
```
The required initial velocity is 49.04999999999815 m/s
```

Eigenvalue problems

$$-\frac{\hbar}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi,$$
$$\psi(x=0) = \psi(x=L) = 0.$$

- Shooting method does not work for finding wavefunctions that satisfy two boundary conditions, as in QM square well, except for valid eigenvalues E.

- So for these problems, E is the parameter that must be varied instead of the leftmost slope of wavefunction.



A word on stability

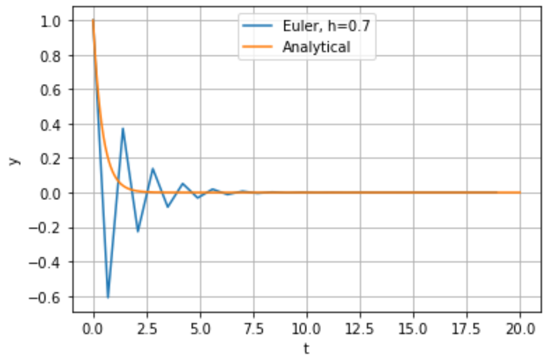
- We have focused on accuracy and speed in investigating our solutions to ODEs.
- But stability is also important!
- The stability of solutions tells us how fast initially close solutions diverge from each other.

- Some systems are inherently unstable and so will always be challenging to simulate. Physical stability or instability of a system can be determined from small perturbations to a solution of the ODE.
- But even for physically stable systems, numerical methods can be unstable and give truncation errors that grow.
- Example: $y'(t) = -2.3y(t)$, $y(t=0) = 1$ is a stable system (tends to a finite number).
  - Solution $y(t) = \exp(-2.3t) : y \to 0$ as $t \to \infty$
  - Forward Euler stable for $h = 0.7$ but unstable for $h = 1$.

In [46]:
```
import matplotlib.pyplot as plt
import numpy as np

y0 = 1.
a = 0.
b = 20.
h = 0.7 # vary this
N = int((b-a)/h)
y = np.empty(N)
time = np.zeros(N)

y[0] = y0
for k in range(1, N):
    time[k] = k*h
    y[k] = y[k-1] + h*(-2.3*y[k-1])  # Euler time step

t_a = np.linspace(a,b,10000)
y_a = np.exp(-2.3*t_a)  # analytical solution for plotting
```

In [47]:
```
plt.plot(time, y, label='Euler, h={0:.1f}'.format(h))
plt.plot(t_a, y_a, label='Analytical')
plt.xlabel('t')
plt.ylabel('y')
plt.grid()
plt.legend(loc='upper center')
```

Out[47]: `<matplotlib.legend.Legend at 0x7efc8dca2c10>`



Why is forward Euler unstable in some cases?

- Explicitly write the solution: for each time step,
$$y_{k+1} = y_k + h_k \lambda y_k \qquad \text{(here, } \lambda = -2.3\text{)}$$
- And for k time steps,
$$y_k = (1 + h_k \lambda)^k y_0.$$
- For the method to be stable, the magnitude of growth factor
$$|1 + h_k \lambda| \leq 1 \quad \Rightarrow \quad \lambda < 0,\ h_k \leq |2/\lambda|.$$

We will investigate more of this in the coming labs.

Summary

- Adaptive RK4: do two RK4 steps, compute error, adjust step size.
    - More operations "per step", but gains can be significant if function varies in concentrated regions.
- MMP: a way to make the error even globally (not trivial).
- Bulirsch-Stoer: use MMP to kill even orders of error, one by one.
- BVPs shooting method: combine ODE integration with root finding
    - eigenvalue problems: it's the eigenvalue, not the initial or boundary value, that we try varying.